

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
 Data File : BG061180.D
 Acq On : 13 May 2024 18:08
 Operator : MA/JU
 Sample : P2454-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SP25-06-20240510-WC

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061180.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.150	21	27	47	rVB	720311	1721472	5.45%	0.519%
2	5.524	424	431	439	rBV	316000	542687	1.72%	0.164%
3	7.110	693	701	709	rBV	219553	390641	1.24%	0.118%
4	9.084	1031	1037	1046	rVB	391535	745936	2.36%	0.225%
5	10.724	1312	1316	1324	rVB2	208223	388533	1.23%	0.117%
6	11.205	1392	1398	1402	rBV	188363	316455	1.00%	0.095%
7	11.963	1522	1527	1531	rBV	241929	376577	1.19%	0.114%
8	12.492	1612	1617	1628	rVV2	268902	629054	1.99%	0.190%
9	12.998	1688	1703	1715	rBV4	937162	4019253	12.72%	1.212%
10	13.180	1730	1734	1741	rVB	869263	1368505	4.33%	0.413%
11	13.614	1802	1808	1814	rVB3	584716	1147099	3.63%	0.346%
12	13.726	1821	1827	1833	rVB	888357	1446869	4.58%	0.436%
13	13.938	1855	1863	1866	rBV4	716580	1712651	5.42%	0.516%
14	14.037	1874	1880	1887	rBV3	1004253	2161882	6.84%	0.652%
15	14.149	1891	1899	1904	rVB	952788	2150759	6.81%	0.649%
16	14.331	1926	1930	1933	rBV	974428	1323065	4.19%	0.399%
17	14.502	1956	1959	1964	rBV2	406049	607009	1.92%	0.183%
18	14.613	1973	1978	1982	rVB2	323910	521354	1.65%	0.157%
19	14.737	1992	1999	2011	rVB2	1895096	4667280	14.77%	1.407%
20	14.978	2028	2040	2045	rBV	2131290	4990603	15.80%	1.505%
21	15.030	2045	2049	2052	rVV	1587862	2336058	7.40%	0.704%
22	15.066	2052	2055	2061	rVB	1336904	1755446	5.56%	0.529%
23	15.201	2075	2078	2080	rBV2	340239	441824	1.40%	0.133%
24	15.260	2086	2088	2092	rVB	871055	845376	2.68%	0.255%
25	15.377	2105	2108	2113	rVB	2637340	3810493	12.06%	1.149%
26	15.442	2113	2119	2123	rBV3	780030	1610922	5.10%	0.486%
27	15.536	2128	2135	2139	rVB2	4751507	8511395	26.94%	2.567%
28	15.589	2139	2144	2145	rBV	1216567	1662760	5.26%	0.501%
29	15.618	2145	2149	2162	rVB2	5741197	12133717	38.41%	3.659%
30	15.747	2167	2171	2174	rBV	996684	1413456	4.47%	0.426%
31	15.794	2175	2179	2180	rBV3	498654	700189	2.22%	0.211%
32	15.865	2183	2191	2193	rBV2	4983421	11130877	35.24%	3.356%
33	15.929	2198	2202	2205	rVV2	7045380	10230212	32.38%	3.085%
34	15.965	2205	2208	2210	rVV	2576924	3154550	9.99%	0.951%
35	16.000	2210	2214	2219	rVV	5655689	11135922	35.25%	3.358%
36	16.053	2219	2223	2228	rVV	5383019	9923275	31.41%	2.992%

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Instrument :
BNA_G
ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.129	2230	2236	2239	rVV2	7348349	12741960	40.34%	3.842%
38	16.170	2239	2243	2245	rVV3	1846909	3213330	10.17%	0.969%
39	16.241	2247	2255	2260	rVV2	13322907	31589645	100.00%	9.526%
40	16.294	2260	2264	2270	rVB	6928672	12921399	40.90%	3.896%
41	16.405	2276	2283	2286	rBV	7859296	16460582	52.11%	4.964%
42	16.523	2294	2303	2308	rBV2	10755446	26392457	83.55%	7.958%
43	16.593	2308	2315	2317	rBV2	6519952	13093890	41.45%	3.948%
44	16.728	2333	2338	2341	rBV2	4693278	8525044	26.99%	2.571%
45	16.899	2361	2367	2371	rVB	4868440	7721182	24.44%	2.328%
46	16.946	2371	2375	2379	rVB	3762324	5077508	16.07%	1.531%
47	17.005	2379	2385	2391	rBV2	8742099	17206092	54.47%	5.188%
48	17.116	2396	2404	2409	rVV4	7747636	24440244	77.37%	7.370%
49	17.163	2409	2412	2415	rVB	5429517	6966020	22.05%	2.101%
50	17.298	2425	2435	2437	rBV3	7816423	23020466	72.87%	6.942%
51	17.398	2447	2452	2457	rBV4	4605267	10234723	32.40%	3.086%

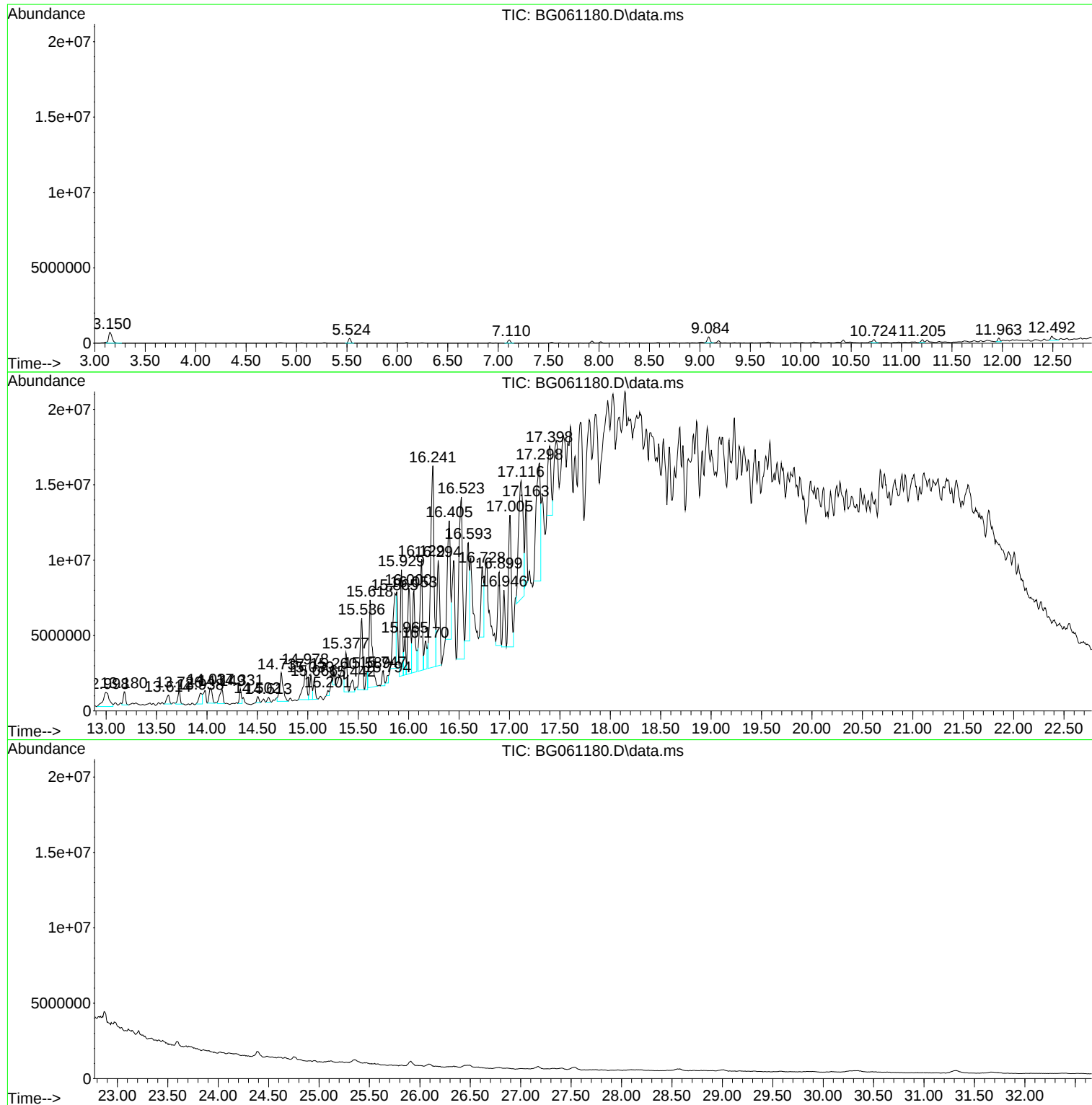
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Sample : P2454-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
SP25-06-20240510-WC

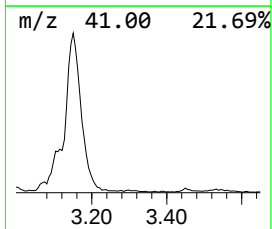
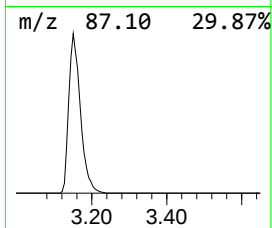
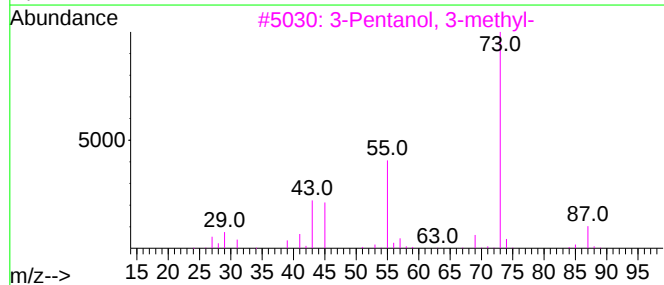
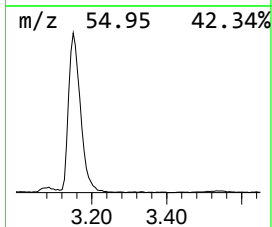
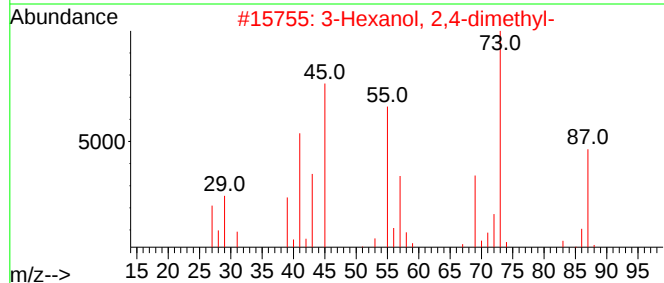
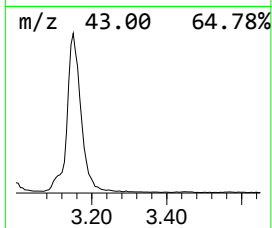
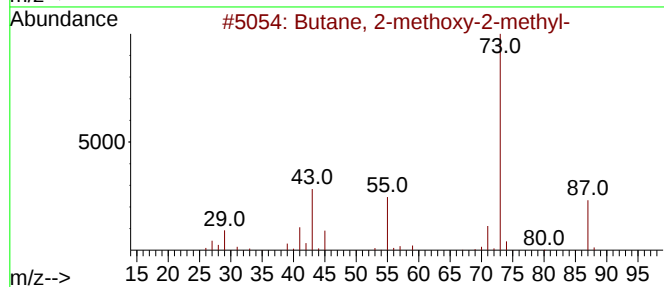
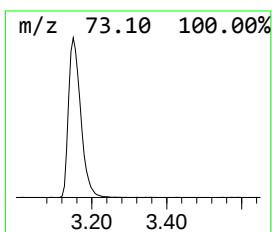
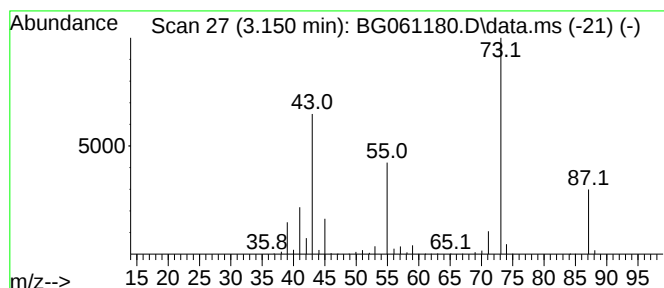
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.150	88.14 ng	1721470	1,4-Dichlorobenzene-d4	7.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	36
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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Misc :
ALS Vial : 9 Sample Multiplier: 1

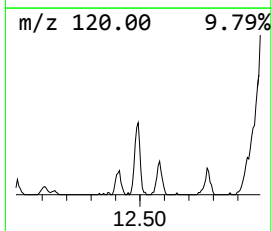
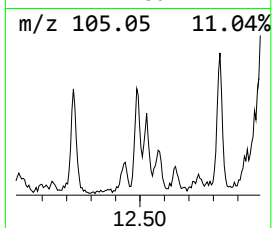
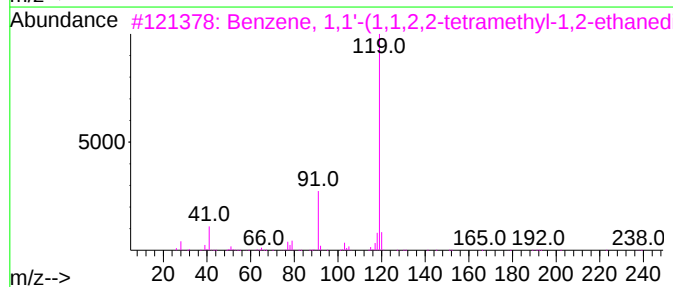
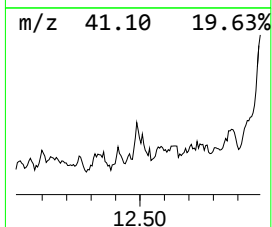
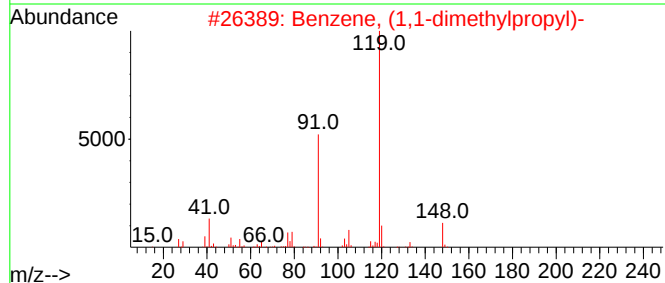
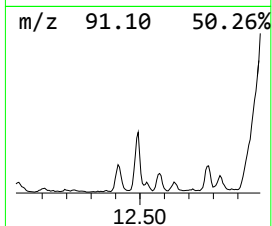
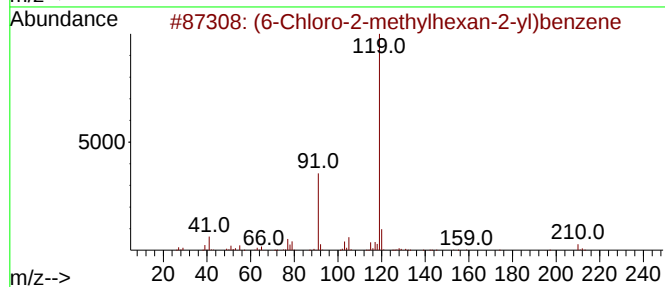
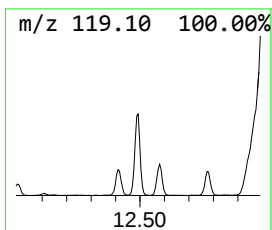
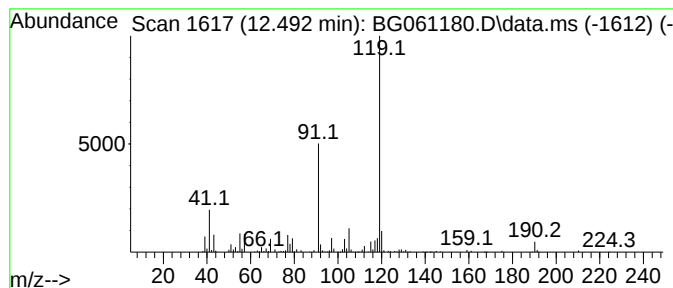
Instrument :
BNA_G
ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (6-Chloro-2-methylhexan-2-yl... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.492	32.38 ng	629054	Naphthalene-d8	10.724	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	86
2	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	78
3	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	72
4	2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	72
5	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	72



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Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

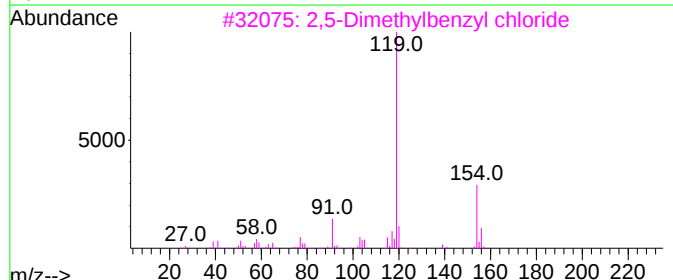
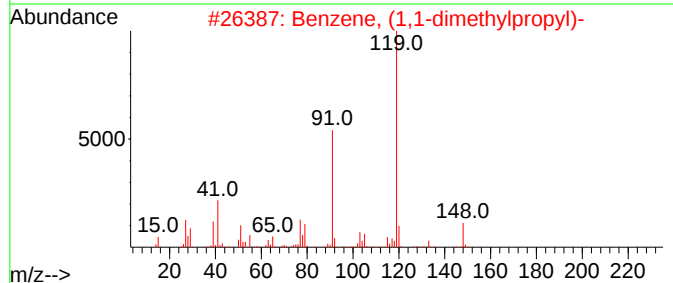
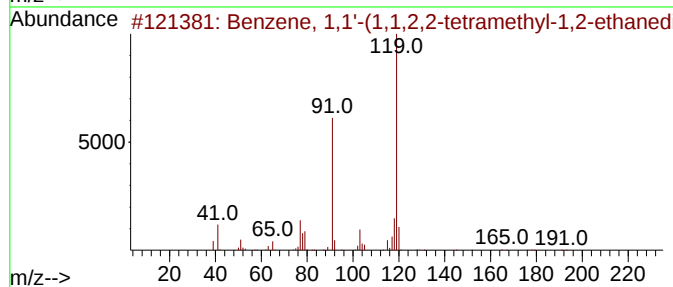
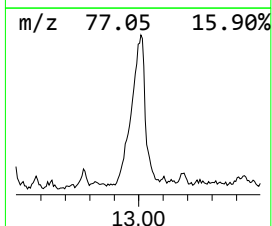
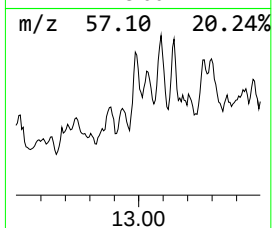
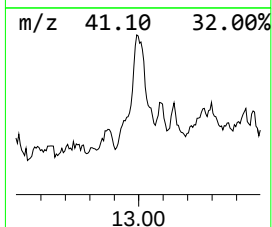
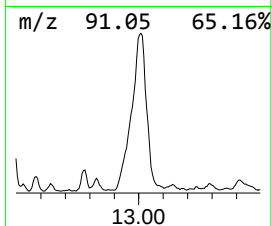
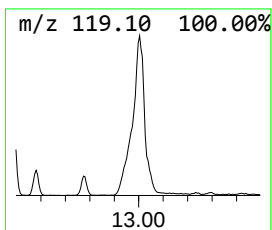
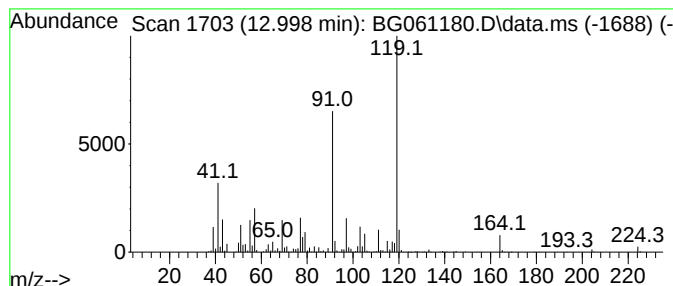
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,1'-(1,1,2,2-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.998	154.19 ng	4019250	Acenaphthene-d10		14.566	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,1,2,2-tetrameth...		238	C18H22	001889-67-4	68
2	Benzene, (1,1-dimethylpropyl)-		148	C11H16	002049-95-8	64
3	2,5-Dimethylbenzyl chloride		154	C9H11Cl	000824-45-3	64
4	Butyric acid, 2-phenyl-, undec-2...		316	C21H32O2	1000406-92-0	64
5	Benzene, tert-butyl-		134	C10H14	000098-06-6	64



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Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

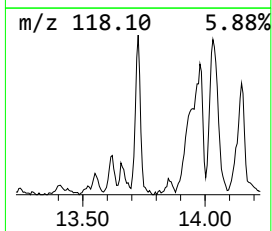
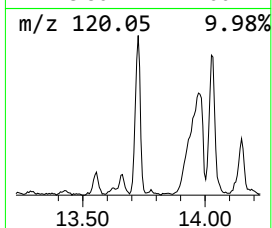
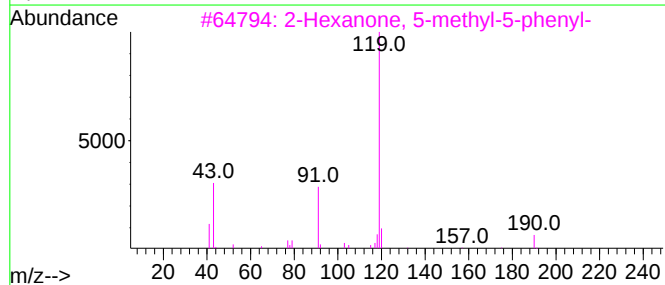
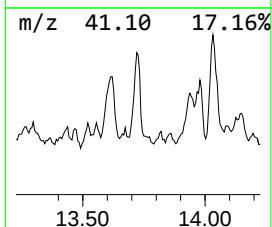
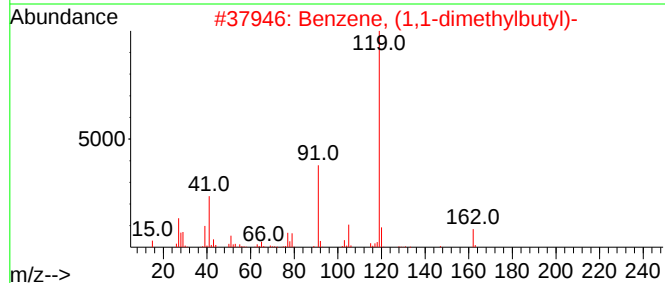
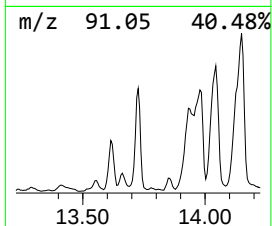
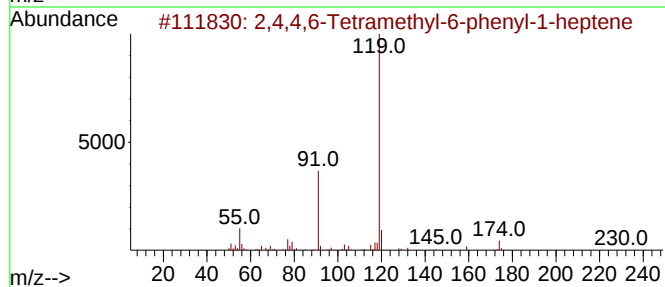
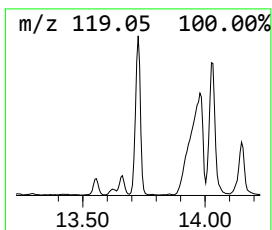
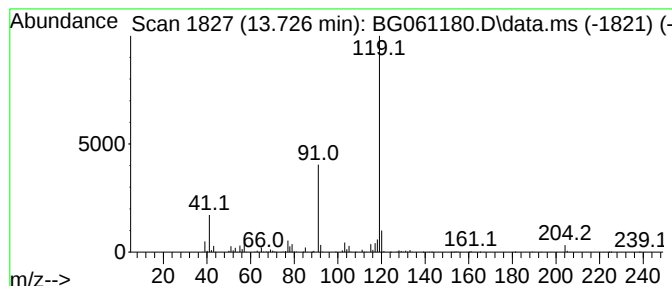
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BNA_G
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,4,4,6-Tetramethyl-6-pheny... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.726	55.50 ng	1446870	Acenaphthene-d10	14.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	83
2	Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	78
3	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	78
4	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	72
5	Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	72



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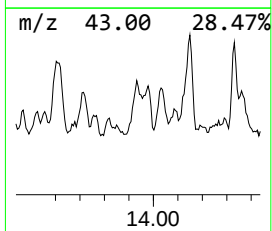
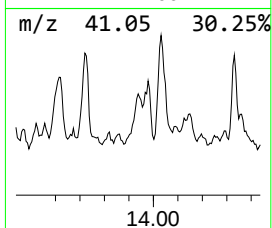
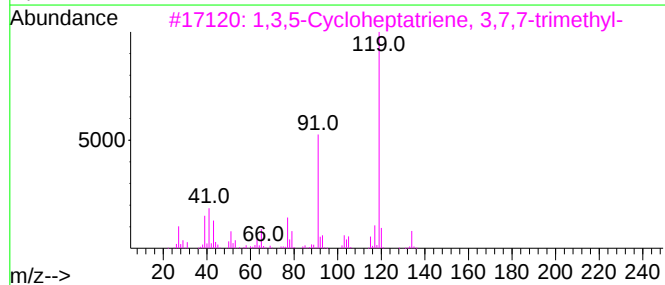
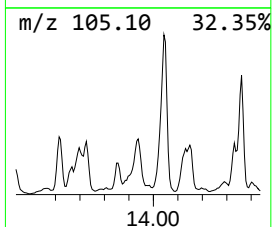
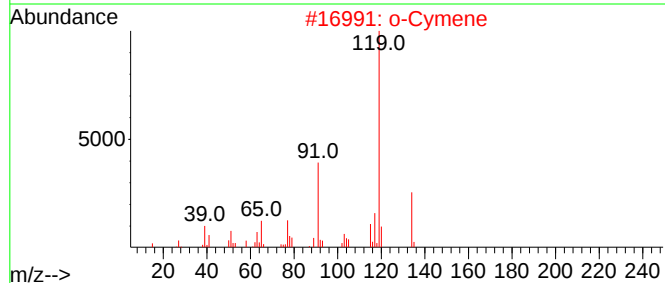
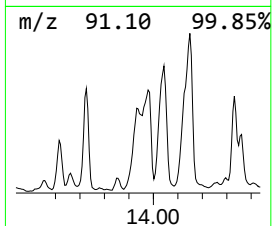
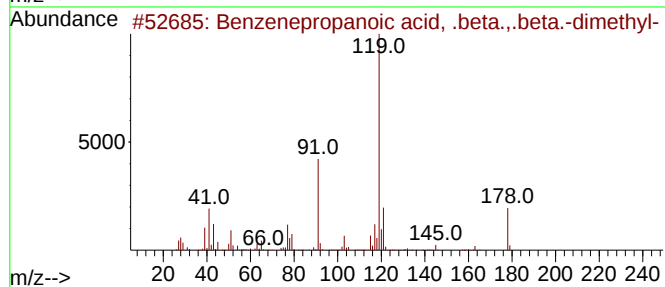
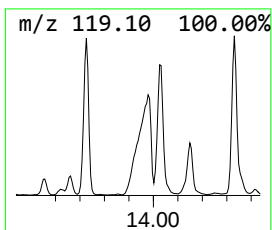
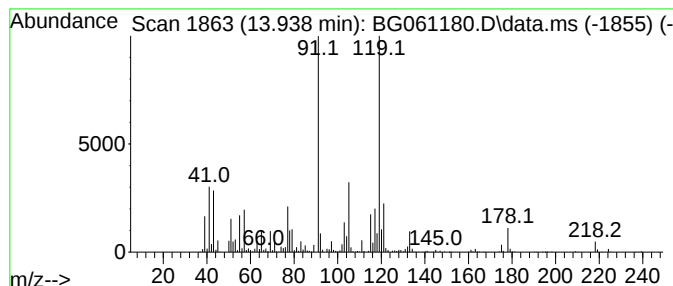
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BNA_G
ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzenepropanoic acid, .bet... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.938	65.70 ng	1712650	Acenaphthene-d10			14.566
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, .beta.,.b...		178	C11H14O2	001010-48-6	76
2	o-Cymene		134	C10H14	000527-84-4	70
3	1,3,5-Cycloheptatriene, 3,7,7-tr...		134	C10H14	003479-89-8	59
4	3,4-Dimethylbenzenacetic acid		164	C10H12O2	017283-16-8	59
5	Benzene, 1-ethyl-3,5-dimethyl-		134	C10H14	000934-74-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP25-06-20240510-WC

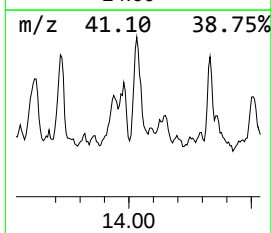
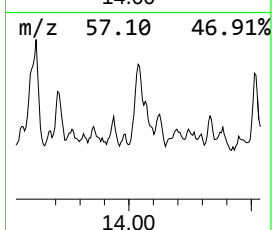
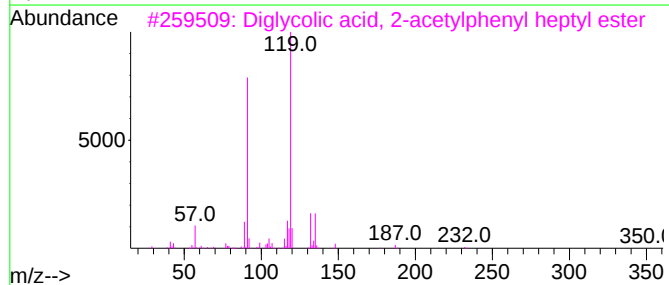
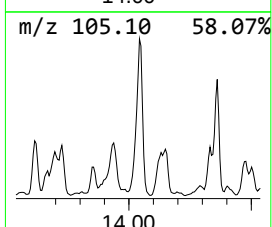
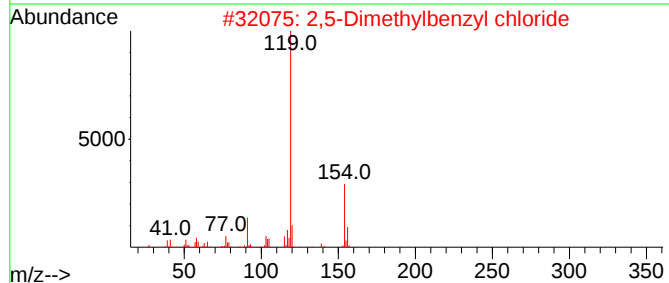
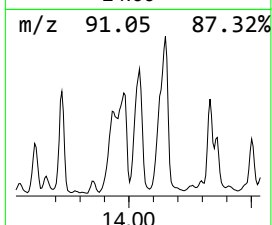
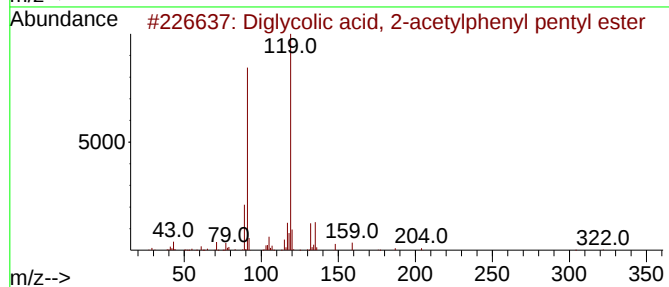
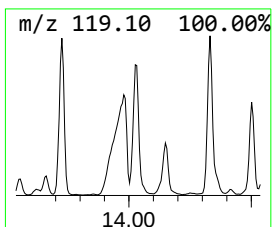
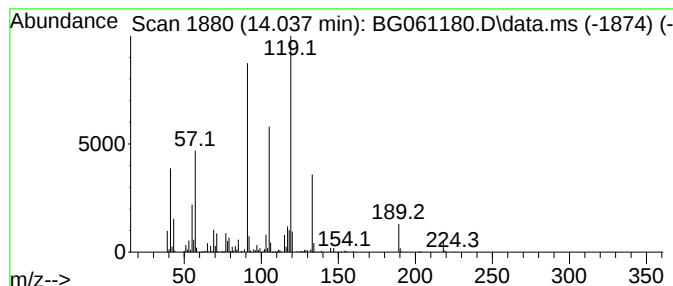
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Diglycolic acid, 2-acetylph... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.038	82.93 ng	2161880	Acenaphthene-d10	14.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diglycolic acid, 2-acetylphenyl ...	322	C17H22O6	1000382-72-0	64
2			2,5-Dimethylbenzyl chloride	154	C9H11Cl	000824-45-3	64
3			Diglycolic acid, 2-acetylphenyl ...	350	C19H26O6	1000382-72-3	59
4			Diglycolic acid, 2-acetylphenyl ...	364	C20H28O6	1000382-72-4	59
5			Diglycolic acid, 2-acetylphenyl ...	392	C22H32O6	1000382-72-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

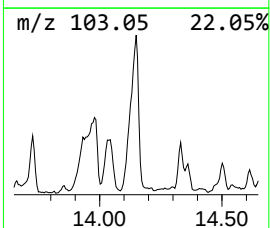
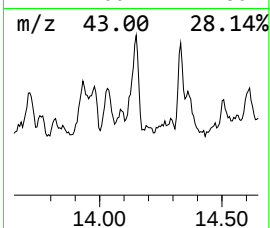
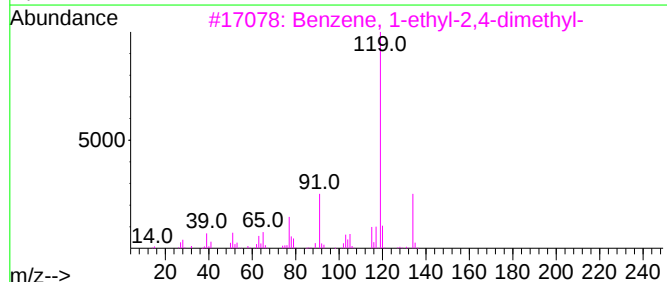
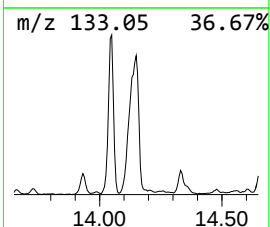
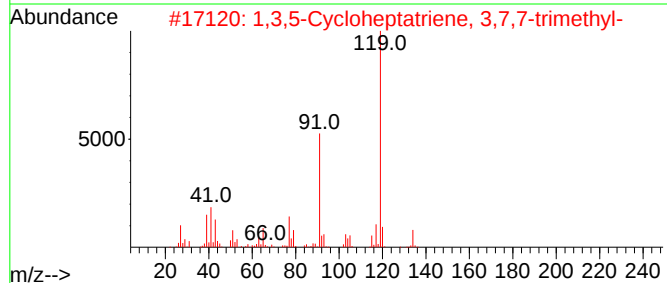
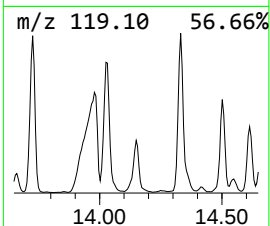
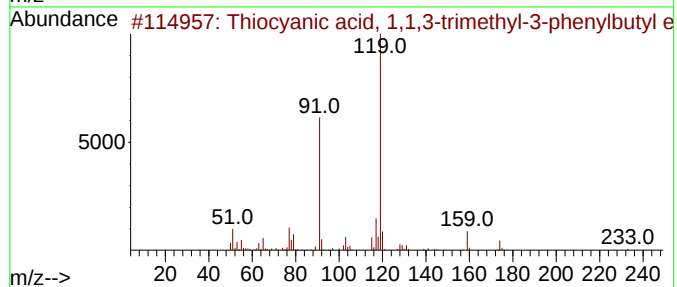
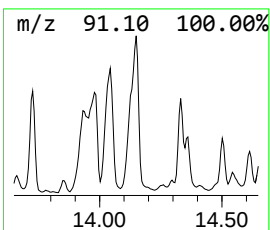
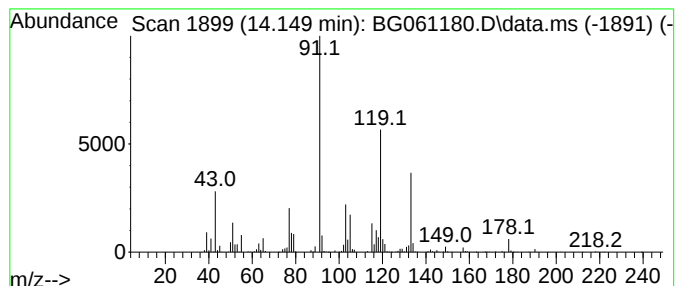
Instrument :
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ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Thiocyanic acid, 1,1,3-trim... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.149	82.51 ng	2150760	Acenaphthene-d10	14.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiocyanic acid, 1,1,3-trimethyl...	233	C14H19NS	1000293-27-7	50
2	1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	50
3	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	49
4	Benzeneacetic acid, .alpha.-ethy...	178	C11H14O2	002294-71-5	47
5	Disiloxane, 1,1,3,3-tetramethyl-	134	C4H14OSi2	003277-26-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

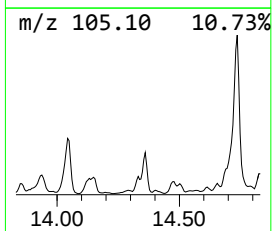
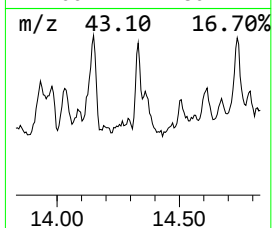
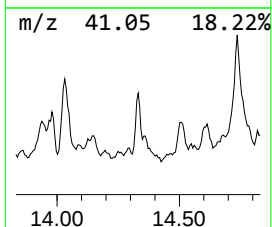
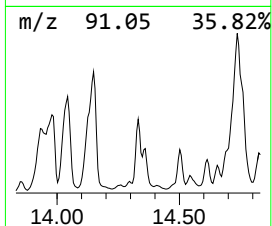
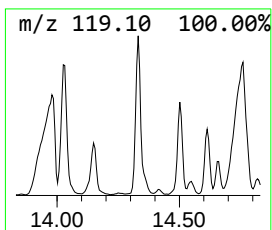
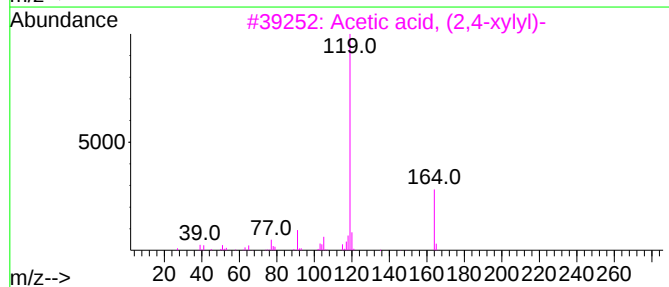
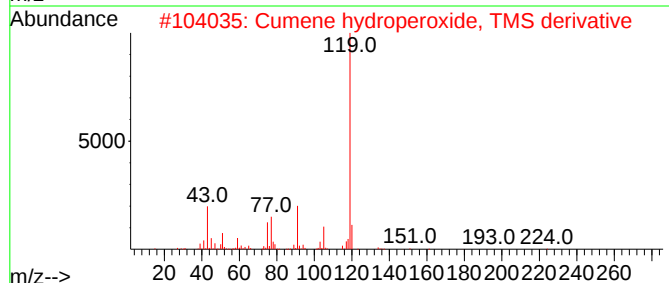
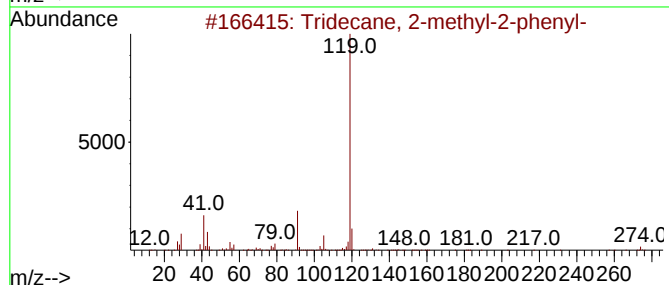
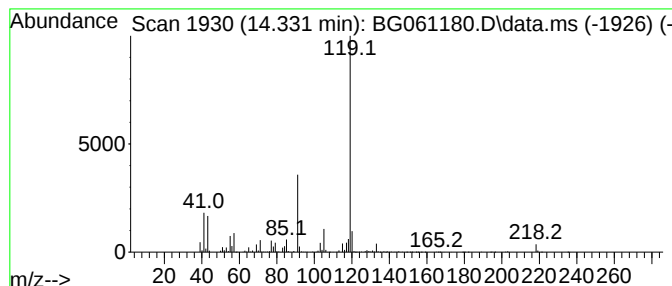
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Tridecane, 2-methyl-2-phenyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.331	50.76 ng	1323070	Acenaphthene-d10	14.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	72
2	Cumene hydroperoxide, TMS deriva...	224	C12H20O2Si	018057-16-4	72
3	Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	72
4	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	72
5	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP25-06-20240510-WC

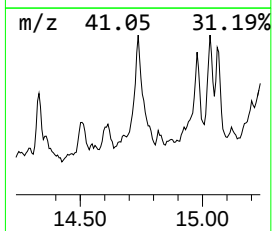
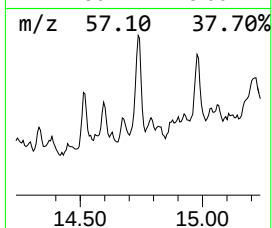
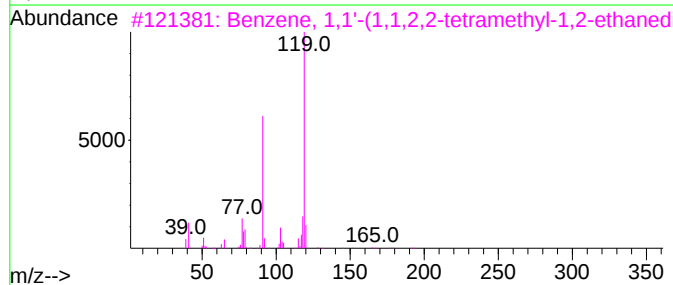
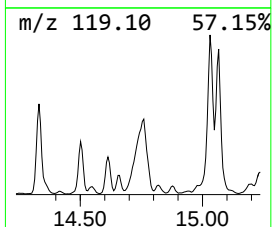
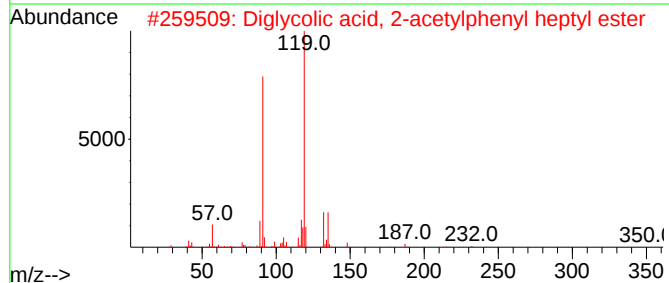
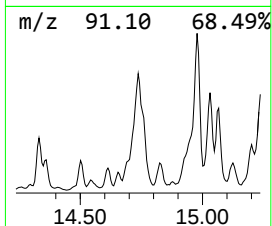
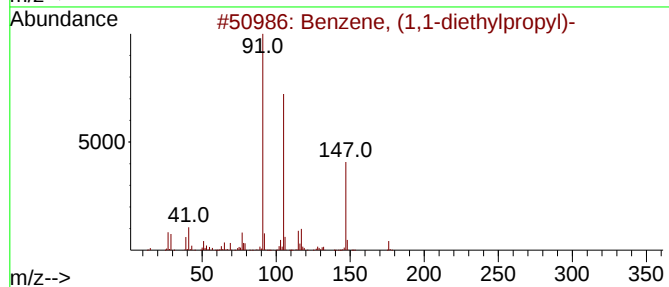
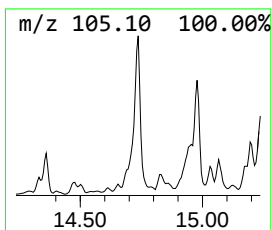
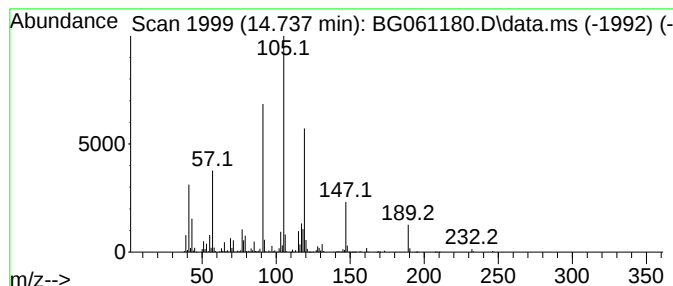
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown14.737 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.737	179.04 ng	4667280	Acenaphthene-d10	14.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-diethylpropyl)-	176	C13H20	004170-84-7	43
2			Diglycolic acid, 2-acetylphenyl ...	350	C19H26O6	1000382-72-3	43
3			Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	38
4			Benzonitrile, 3-ethoxy-	147	C9H9NO	025117-75-3	38
5			7-Methoxymethyl-2,7-dimethylcycl...	164	C11H16O	073992-48-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP25-06-20240510-WC

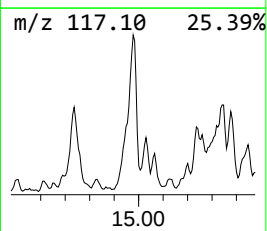
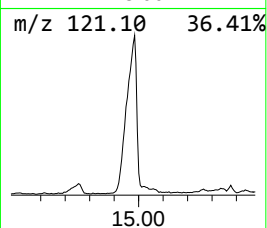
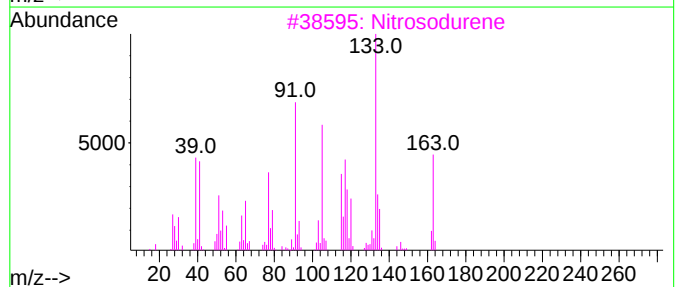
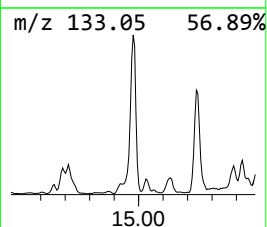
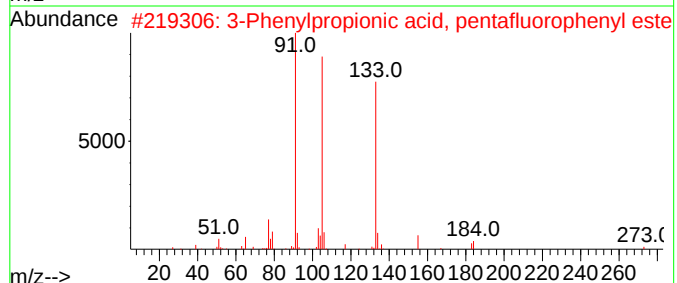
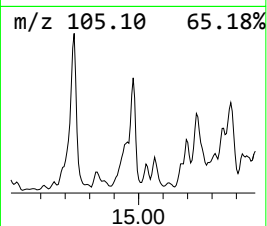
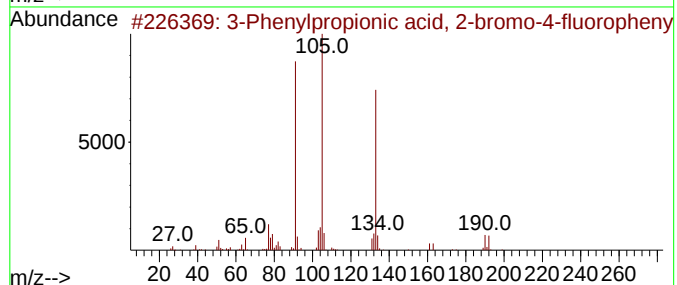
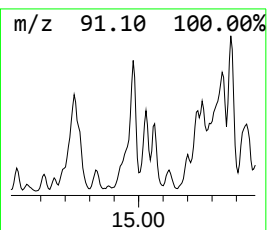
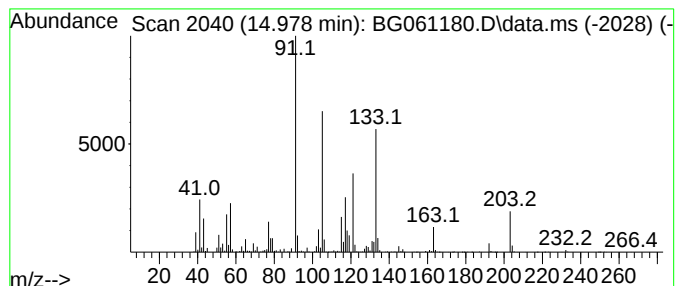
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown14.977 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.977	191.45 ng	4990600	Acenaphthene-d10	14.566

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Phenylpropionic acid, 2-bromo-...	322	C15H12BrF02	1000299-02-3	46
2		3-Phenylpropionic acid, pentaflu...	316	C15H9F5O2	1000354-73-7	43
3		Nitrosodurene	163	C10H13NO	1000430-49-9	38
4		2-Methyl-3-nitrophenyl .beta.-ph...	285	C16H15NO4	040300-01-4	38
5		2-Cyanophenyl .beta.-phenylpropi...	251	C16H13NO2	040123-48-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

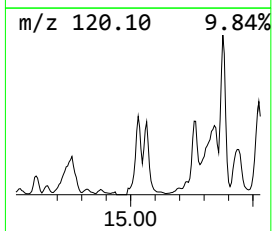
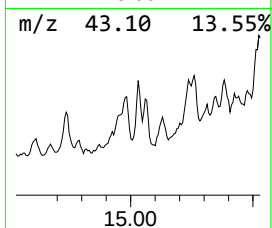
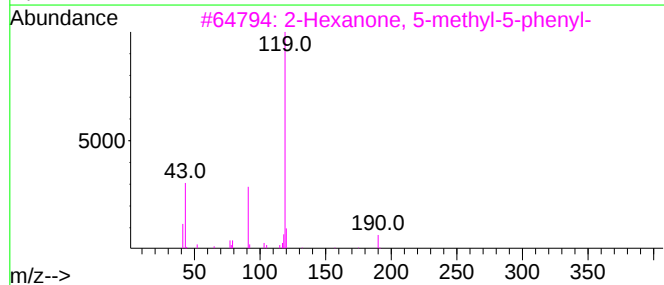
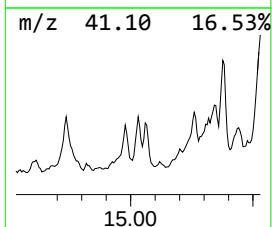
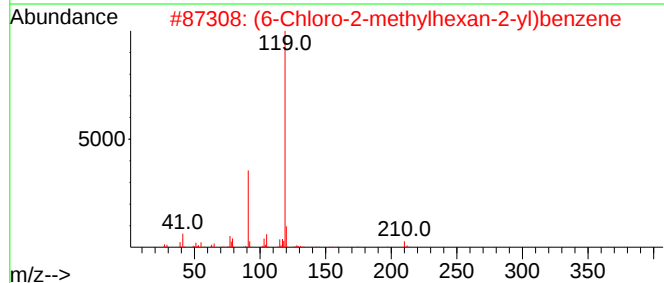
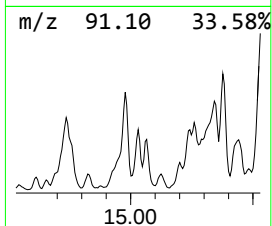
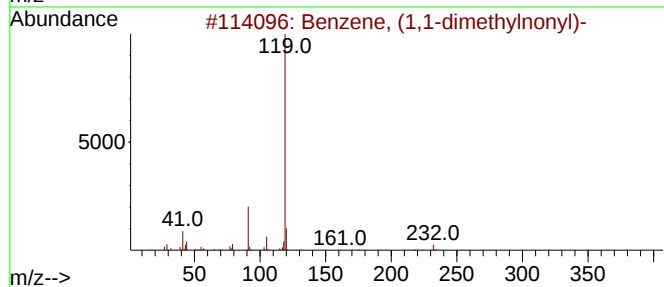
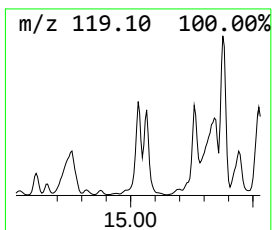
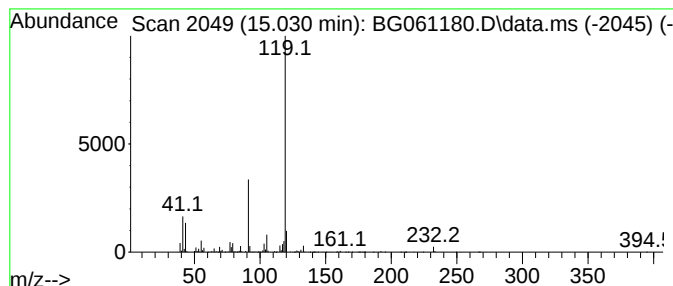
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BNA_G
ClientSampleId :
SP25-06-20240510-WC

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Benzene, (1,1-dimethylnonyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.030	89.61 ng	2336060	Acenaphthene-d10	14.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	86
2	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	86
3	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	78
4	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	78
5	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

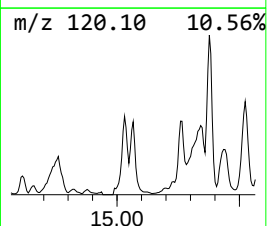
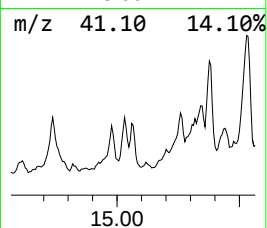
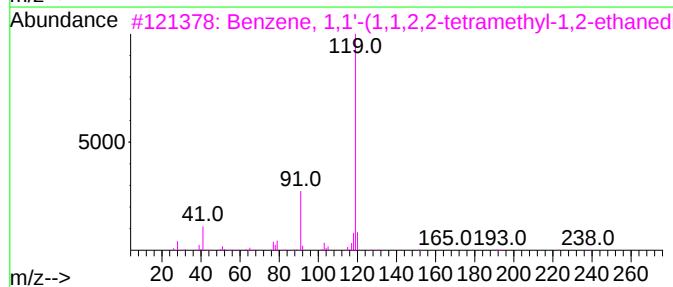
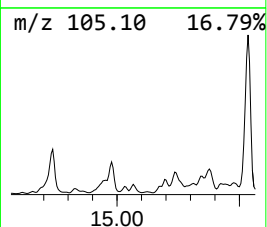
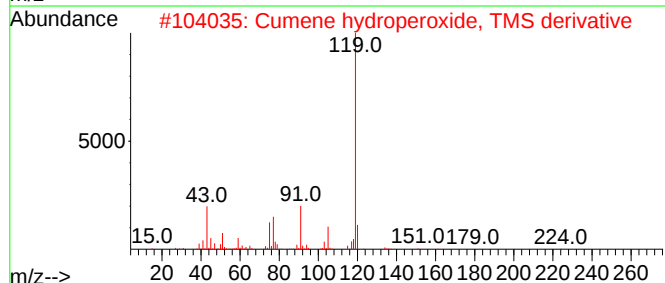
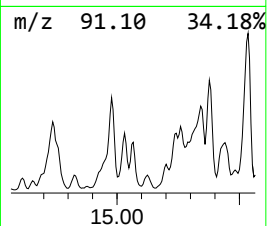
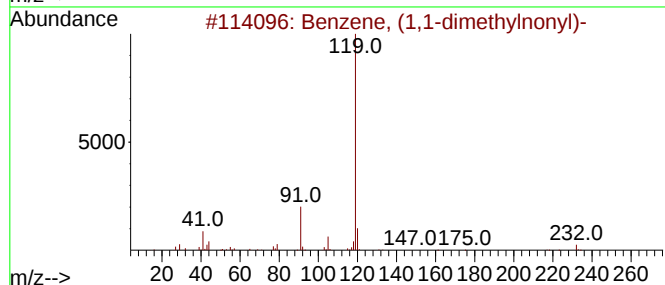
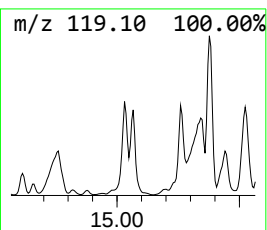
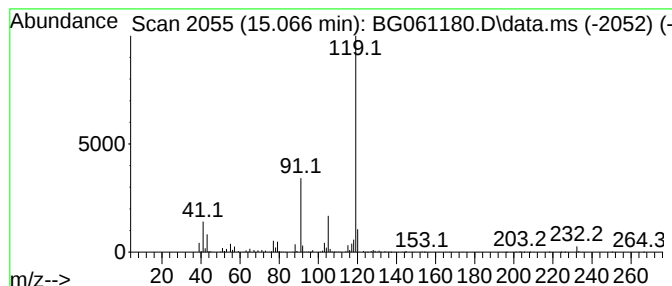
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ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Cumene hydroperoxide, TMS d... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.066	67.34 ng	1755450	Acenaphthene-d10		14.566	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethylnonyl)-		232	C17H28	055191-25-8	80
2	Cumene hydroperoxide, TMS deriva...		224	C12H20O2Si	018057-16-4	72
3	Benzene, 1,1'-(1,1,2,2-tetrameth...		238	C18H22	001889-67-4	72
4	Benzene, (1,1-dimethylpropyl)-		148	C11H16	002049-95-8	72
5	Benzene, (1,1-dimethyldecyl)-		246	C18H30	027854-40-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

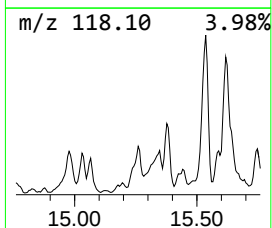
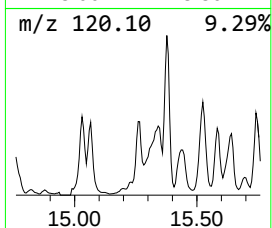
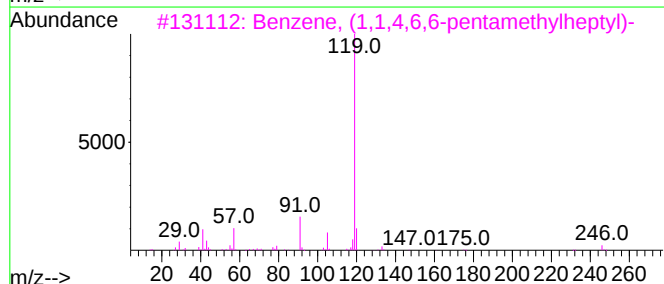
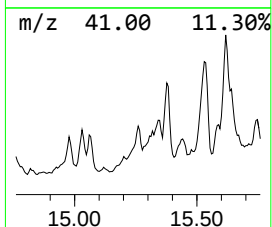
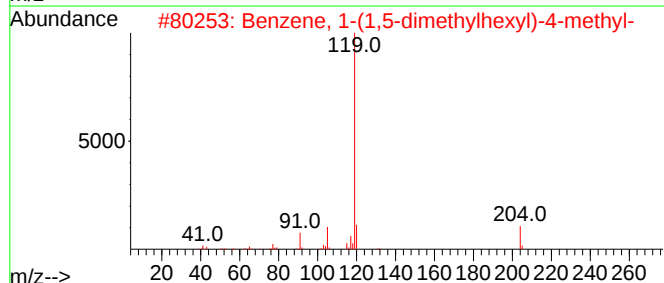
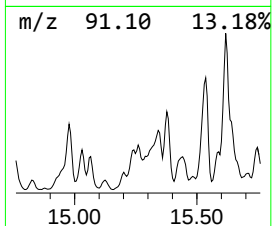
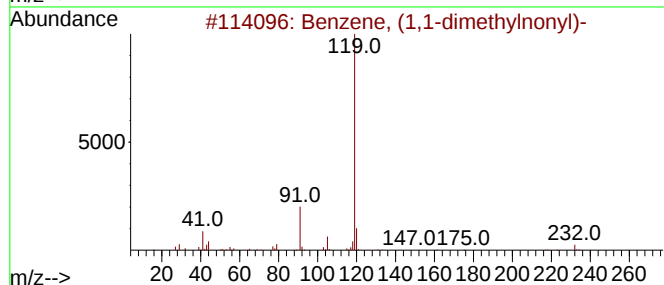
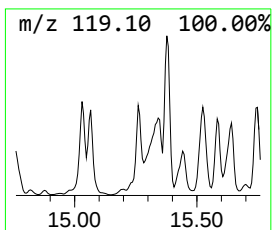
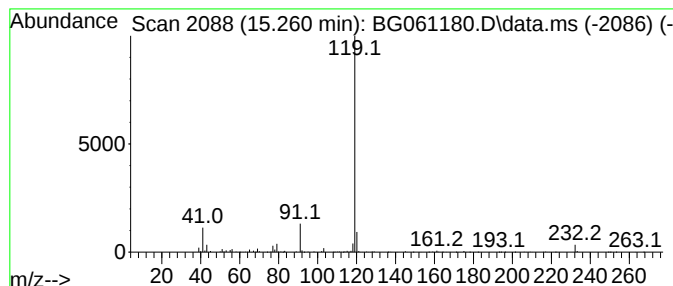
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Benzene, 1-(1,5-dimethylhex... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.260	32.43 ng	845376	Acenaphthene-d10	14.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	86
2	Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	72
3	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	72
4	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	64
5	1,2-Benzenediol, o-(3-cyclopenty...	352	C22H24O4	1000325-95-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

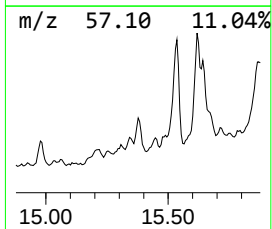
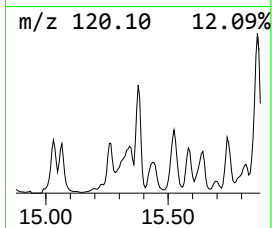
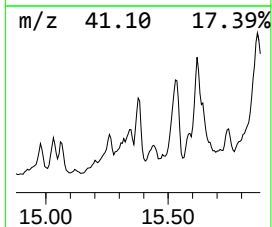
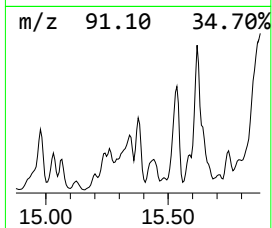
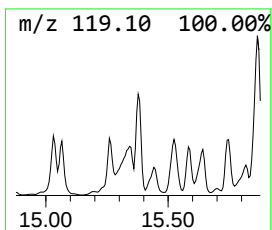
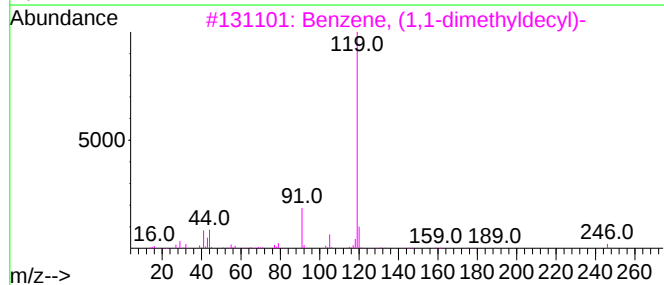
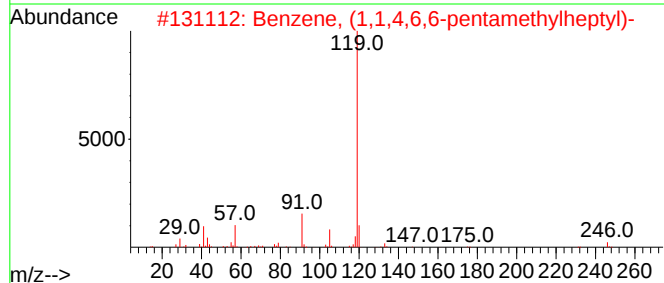
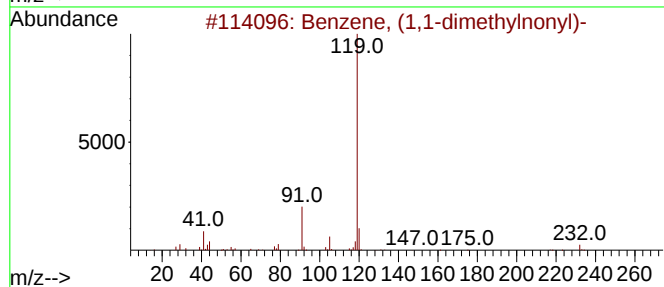
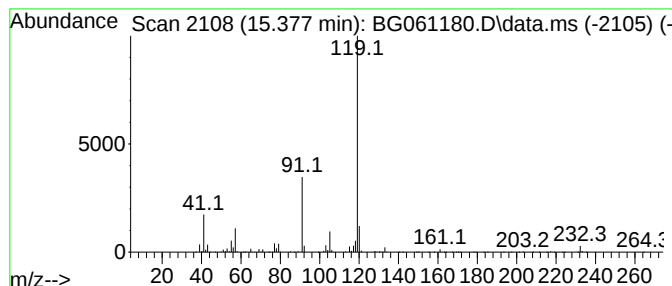
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Benzene, (1,1,4,6,6-pentame... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.377	146.18 ng	3810490	Acenaphthene-d10		14.566	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethylnonyl)-		232	C17H28	055191-25-8	87
2	Benzene, (1,1,4,6,6-pentamethylh...		246	C18H30	055134-07-1	83
3	Benzene, (1,1-dimethyldecyl)-		246	C18H30	027854-40-6	72
4	Benzene, (1,1-dimethylpropyl)-		148	C11H16	002049-95-8	72
5	Pentadecane, 2-methyl-2-phenyl-		302	C22H38	029138-94-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

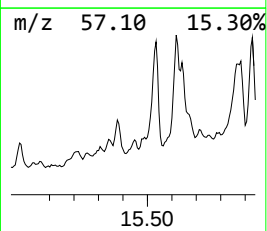
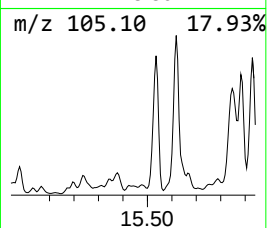
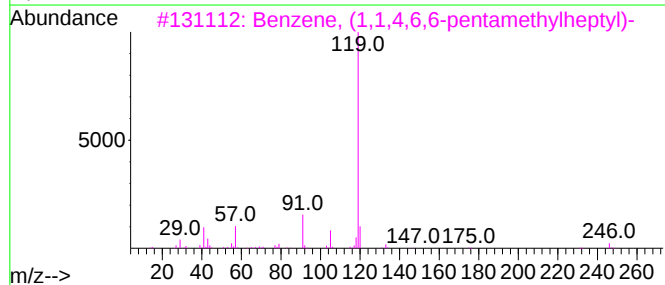
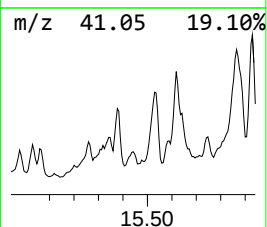
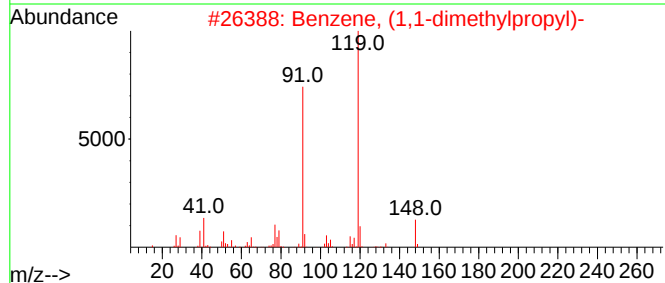
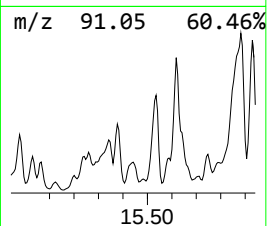
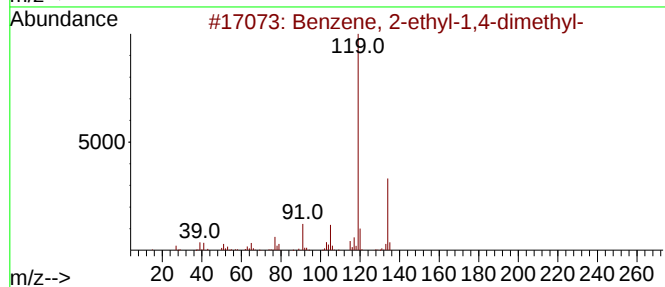
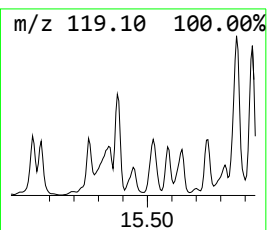
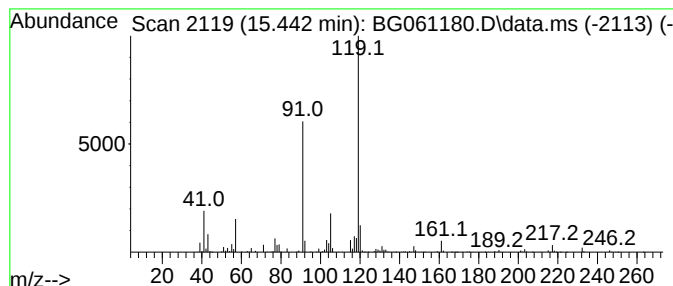
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.442	61.80 ng	1610920	Acenaphthene-d10	14.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	78
2	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	72
3	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	72
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	72
5	Butyric acid, 2-phenyl-, 3-methy...	232	C15H20O2	1000406-91-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP25-06-20240510-WC

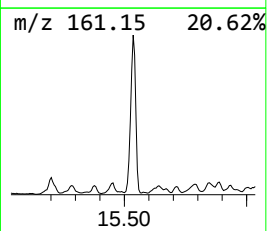
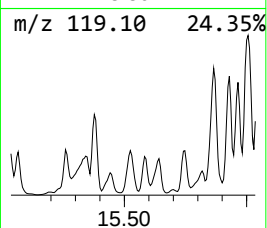
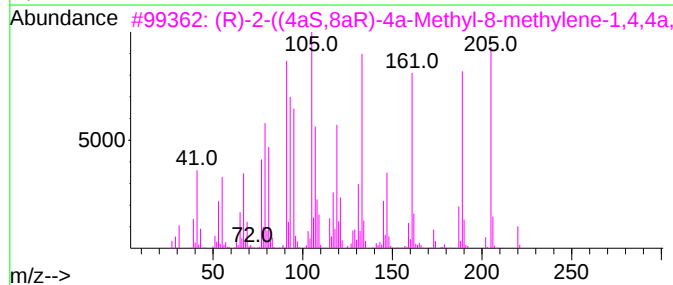
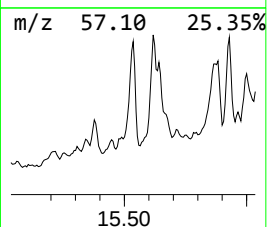
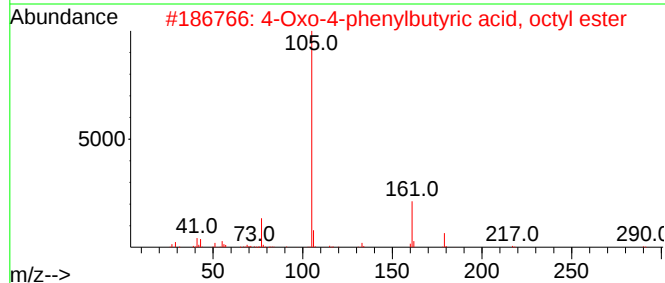
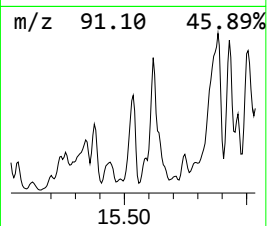
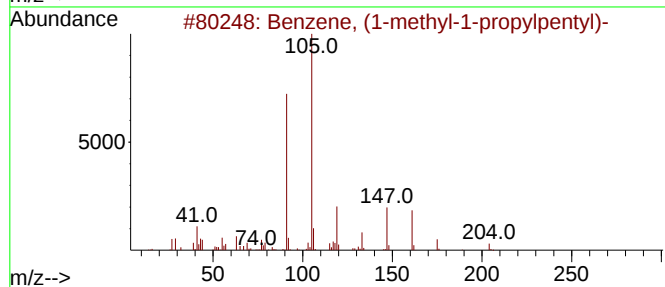
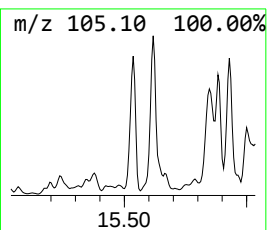
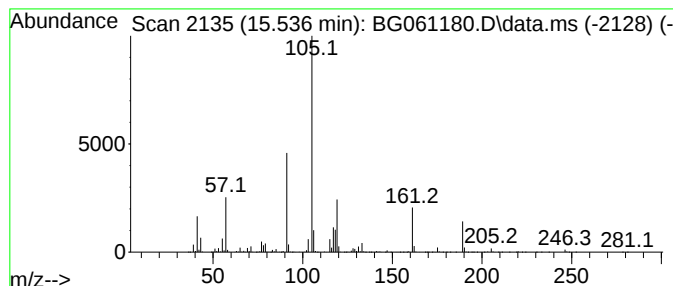
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown15.536 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.536	326.51 ng	8511400	Acenaphthene-d10	14.566

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-methyl-1-propylpentyl)-	204	C15H24	054932-91-1	33
2		4-Oxo-4-phenylbutyric acid, octy...	290	C18H26O3	1010405-97-9	25
3		(R)-2-((4aS,8aR)-4a-Methyl-8-met...	220	C15H24O	028102-68-3	25
4		4-Oxo-4-phenylbutyric acid, tetr...	374	C24H38O3	1000405-98-5	25
5		4-Oxo-4-phenylbutyric acid, decy...	318	C20H30O3	1000405-98-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
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Sample : P2454-01
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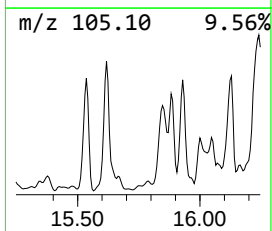
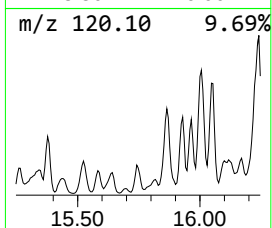
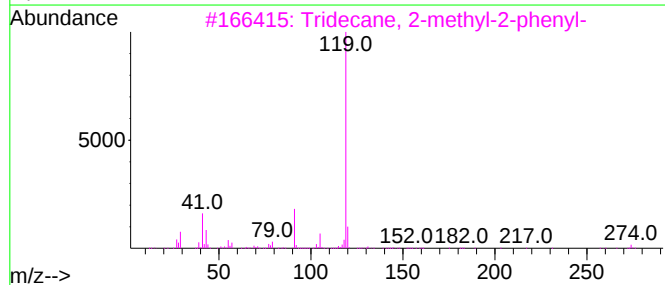
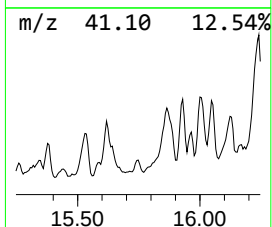
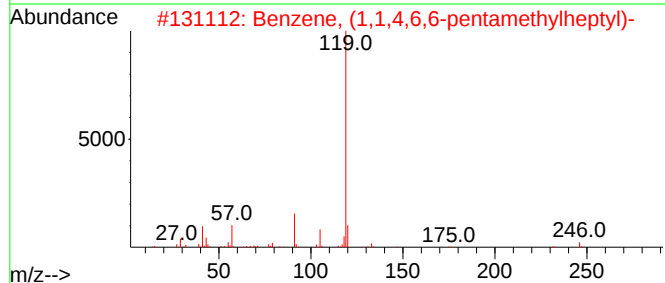
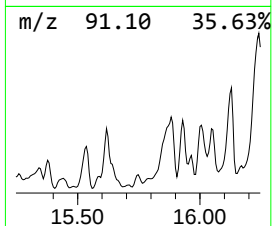
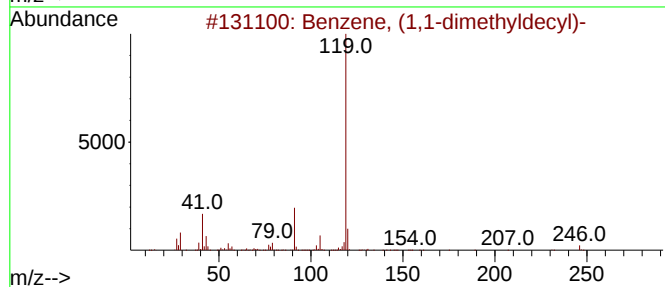
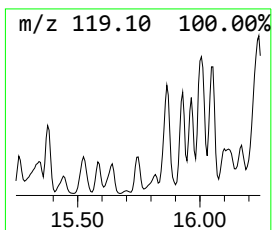
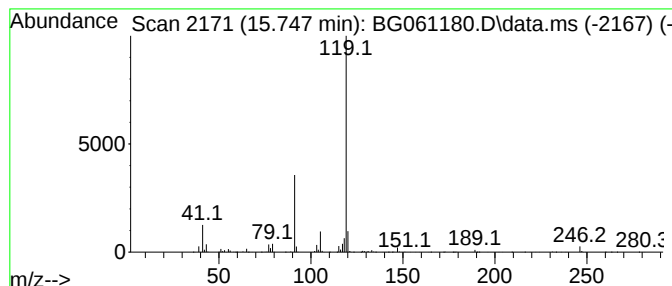
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Benzene, (1,1-dimethyldecyl)- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.747	54.22 ng	1413460	Acenaphthene-d10	14.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	90
2	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	86
3	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	78
4	Cumene hydroperoxide, TMS deriva...	224	C12H20O2Si	018057-16-4	78
5	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

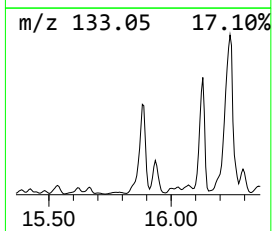
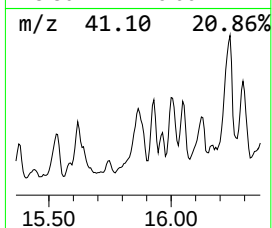
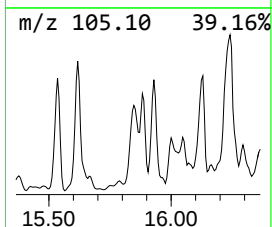
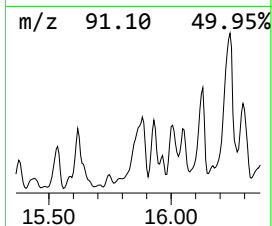
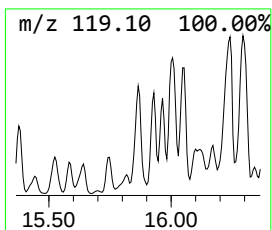
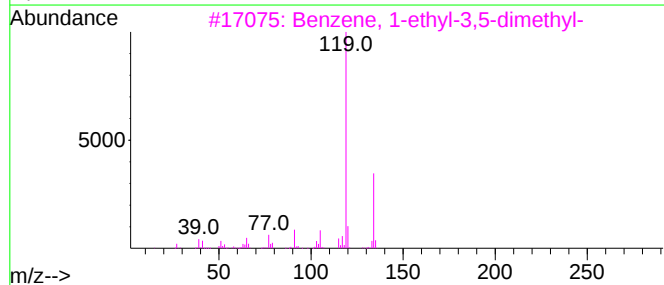
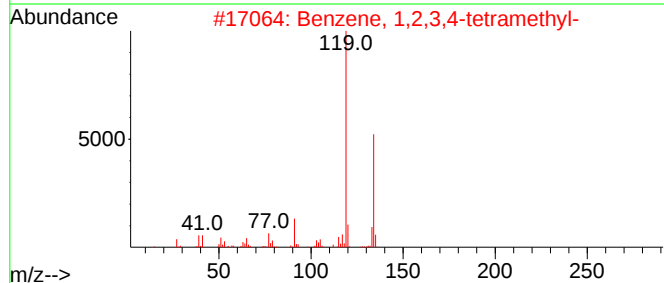
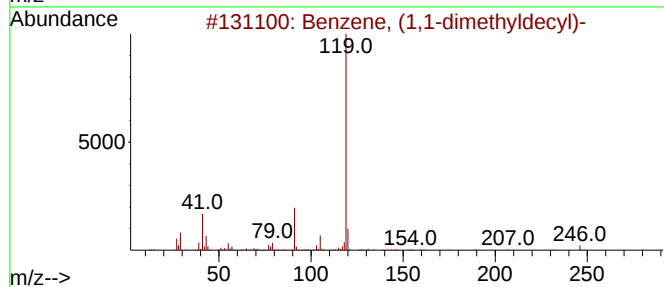
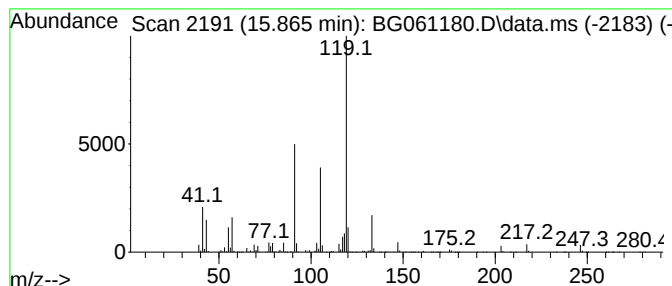
Instrument :
BNA_G
ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.865	427.00 ng	11130900	Acenaphthene-d10	14.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	72
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64
3	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	64
4	1-p-Tolyl-2-(4H-[1,2,4]triazol-3...	233	C11H11N3OS	326888-02-2	64
5	2-Methyl-6-(p-tolyl)hept-2-en-4-ol	218	C15H22O	038142-57-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP25-06-20240510-WC

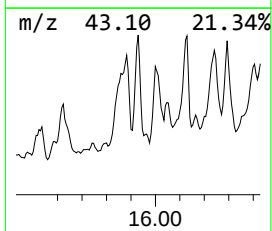
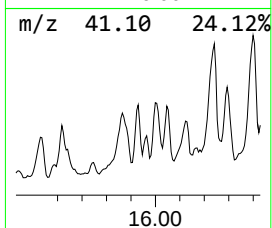
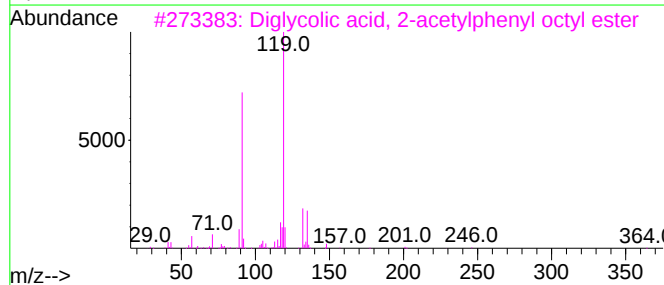
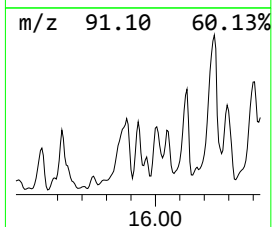
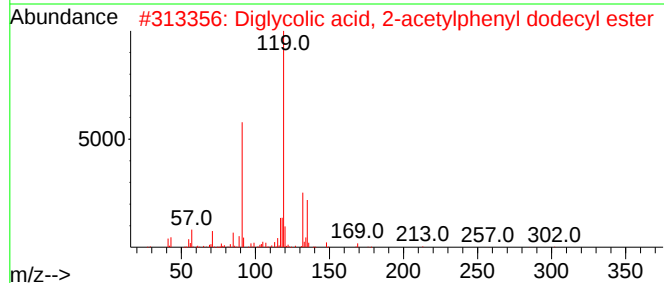
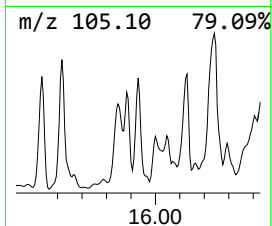
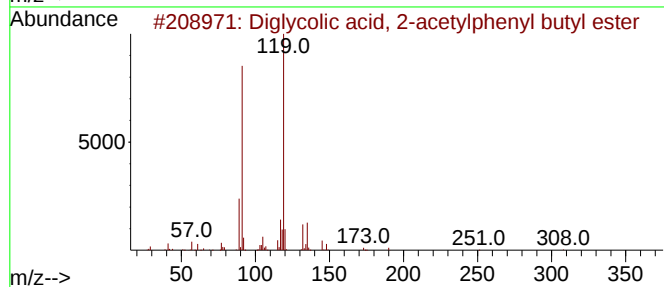
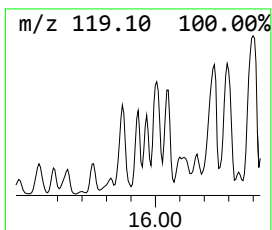
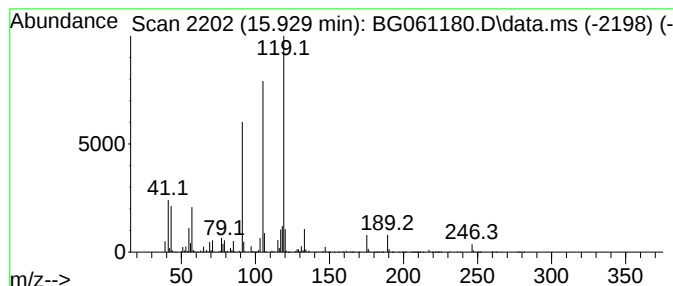
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Diglycolic acid, 2-acetylph... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.929	392.45 ng	10230200	Acenaphthene-d10	14.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diglycolic acid, 2-acetylphenyl ...	308	C16H20O6	1000382-71-9	53
2			Diglycolic acid, 2-acetylphenyl ...	420	C24H36O6	1010382-72-8	53
3			Diglycolic acid, 2-acetylphenyl ...	364	C20H28O6	1000382-72-4	53
4			1,3-Dioxolan-2-one, 4-methyl-5-m...	246	C15H18O3	1000319-92-8	52
5			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

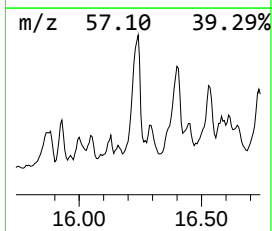
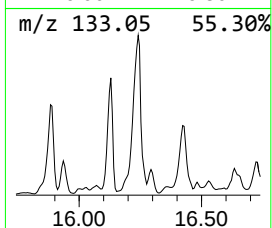
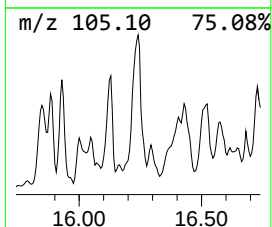
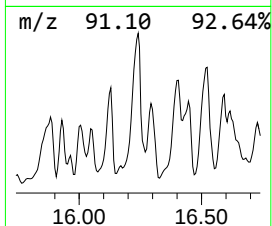
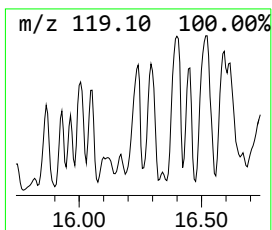
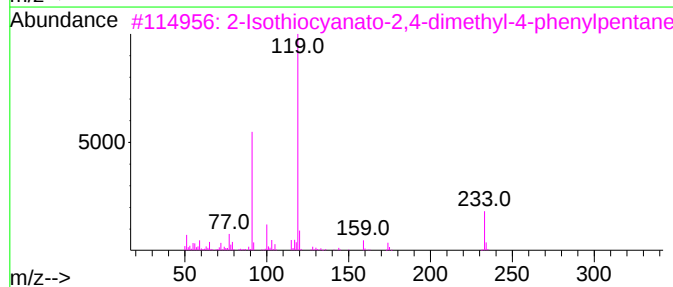
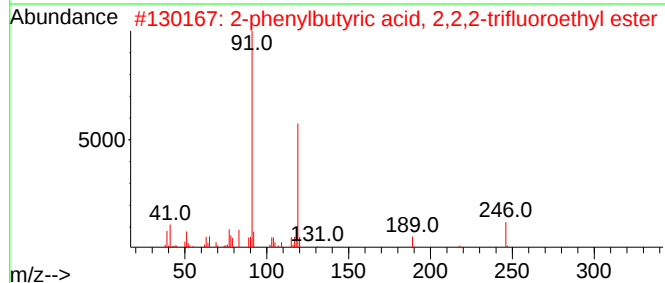
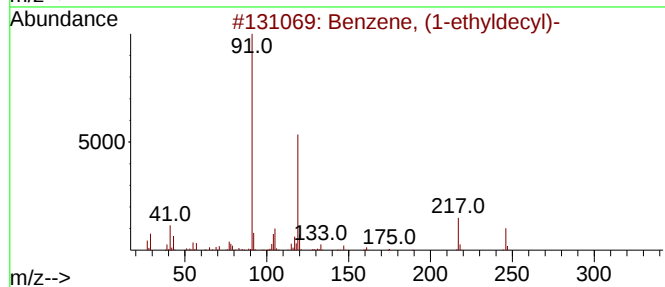
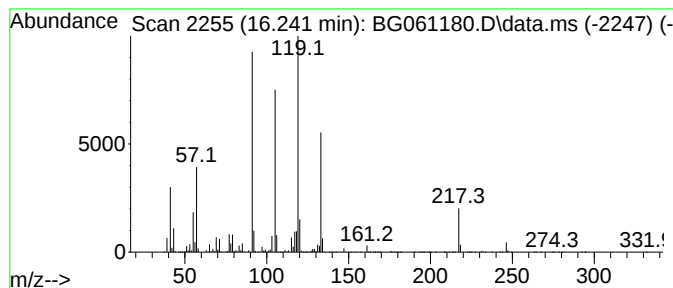
Instrument :
BNA_G
ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Benzene, (1-ethyldecyl)- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.241	27.44 ng	31589600	Phenanthrene-d10	17.345
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, (1-ethyldecyl)-	246 C18H30	002400-00-2 81
2		2-phenylbutyric acid, 2,2,2-trif...	246 C12H13F3O2	1000376-55-3 58
3		2-Isothiocyanato-2,4-dimethyl-4-...	233 C14H19NS	1000293-27-6 47
4		Butyric acid, 2-phenyl-, 3-chlor...	274 C16H15ClO2	1000406-86-3 43
5		o-Cymene	134 C10H14	000527-84-4 43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061180.D
Acq On : 13 May 2024 18:08
Operator : MA/JU
Sample : P2454-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.150	88.1	ng	1721470	1	7.933	390641	20.0
(6-Chloro-2-met...	12.492	32.4	ng	629054	2	10.724	388533	20.0
Benzene, 1,1'-(...	12.998	154.2	ng	4019250	3	14.566	521354	20.0
2,4,4,6-Tetrame...	13.726	55.5	ng	1446870	3	14.566	521354	20.0
Benzenepropanoi...	13.938	65.7	ng	1712650	3	14.566	521354	20.0
Diglycolic acid...	14.038	82.9	ng	2161880	3	14.566	521354	20.0
Thiocyanic acid...	14.149	82.5	ng	2150760	3	14.566	521354	20.0
Tridecane, 2-me...	14.331	50.8	ng	1323070	3	14.566	521354	20.0
unknown14.737	14.737	179.0	ng	4667280	3	14.566	521354	20.0
unknown14.977	14.977	191.4	ng	4990600	3	14.566	521354	20.0
Benzene, (1,1-d...	15.030	89.6	ng	2336060	3	14.566	521354	20.0
Cumene hydroper...	15.066	67.3	ng	1755450	3	14.566	521354	20.0
Benzene, 1-(1,5...	15.260	32.4	ng	845376	3	14.566	521354	20.0
Benzene, (1,1,4...	15.377	146.2	ng	3810490	3	14.566	521354	20.0
Benzene, 2-ethy...	15.442	61.8	ng	1610920	3	14.566	521354	20.0
unknown15.536	15.536	326.5	ng	8511400	3	14.566	521354	20.0
Benzene, (1,1-d...	15.747	54.2	ng	1413460	3	14.566	521354	20.0
Benzene, 1,2,3,...	15.865	427.0	ng	11130900	3	14.566	521354	20.0
Diglycolic acid...	15.929	392.4	ng	10230200	3	14.566	521354	20.0
Benzene, (1-eth...	16.241	27.4	ng	31589600	4	17.345	23020500	20.0