

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
 Data File : BG060215.D
 Acq On : 3 Jan 2024 5:58
 Operator : MA/JU
 Sample : 05899-19
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-07-0-2

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-BG122923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060215.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.126	170	176	184	rVB	95492	150992	1.21%	0.212%
2	5.506	404	411	419	rBV	3125192	4922890	39.33%	6.903%
3	5.571	419	422	430	rVB2	92440	182198	1.46%	0.255%
4	5.947	480	486	494	rBV3	116508	211984	1.69%	0.297%
5	7.099	674	682	697	rBV	3189986	5472630	43.72%	7.674%
6	7.939	814	825	838	rBV	694982	1272089	10.16%	1.784%
7	9.096	1015	1022	1030	rBV	1770585	3158475	25.23%	4.429%
8	10.741	1291	1302	1307	rBV	1109947	2007474	16.04%	2.815%
9	10.788	1307	1310	1323	rVB	308914	537360	4.29%	0.753%
10	12.398	1576	1584	1594	rVB	348444	585488	4.68%	0.821%
11	12.616	1616	1621	1630	rVB	234709	396071	3.16%	0.555%
12	13.197	1713	1720	1729	rBV	5496240	8639823	69.02%	12.115%
13	13.397	1747	1754	1762	rBV4	92382	197803	1.58%	0.277%
14	13.750	1802	1814	1822	rBV4	68038	217366	1.74%	0.305%
15	13.891	1833	1838	1843	rBV2	135010	214273	1.71%	0.300%
16	13.949	1843	1848	1855	rVB2	109715	187451	1.50%	0.263%
17	14.049	1857	1865	1870	rBV4	79051	128536	1.03%	0.180%
18	14.132	1874	1879	1882	rBV2	90131	130204	1.04%	0.183%
19	14.572	1943	1954	1962	rBV	2190450	3448609	27.55%	4.836%
20	14.866	1996	2004	2007	rBV6	68070	144420	1.15%	0.203%
21	14.972	2017	2022	2028	rBV	175055	281059	2.25%	0.394%
22	15.612	2125	2131	2137	rBV3	127369	220497	1.76%	0.309%
23	15.830	2162	2168	2175	rBV5	61739	133849	1.07%	0.188%
24	15.912	2175	2182	2191	rVV5	76451	166204	1.33%	0.233%
25	16.065	2200	2208	2216	rBV	4626573	7156625	57.17%	10.035%
26	16.305	2240	2249	2255	rVB2	273878	513500	4.10%	0.720%
27	16.858	2335	2343	2353	rBV5	92925	216318	1.73%	0.303%
28	17.069	2371	2379	2384	rBV2	93419	161943	1.29%	0.227%
29	17.322	2416	2422	2427	rBV	2890357	4303665	34.38%	6.035%
30	17.363	2427	2429	2439	rVV	270126	369473	2.95%	0.518%
31	17.451	2439	2444	2449	rVV	482179	732208	5.85%	1.027%
32	17.727	2486	2491	2496	rVB	136877	202929	1.62%	0.285%
33	18.209	2566	2573	2577	rBV3	376962	591629	4.73%	0.830%
34	19.942	2860	2868	2883	rBV	9152657	12518042	100.00%	17.553%
35	21.235	3083	3088	3101	rBV	717567	1176505	9.40%	1.650%
36	21.587	3141	3148	3160	rBV2	2630207	4339690	34.67%	6.085%

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ClientSampleId :
GHL-SS-07-0-2

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-BG122923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.398	3279	3286	3293	rBV4	207361	474389	3.79%	0.665%
38	24.760	3677	3688	3702	rBV	1599158	4578347	36.57%	6.420%
39	25.894	3876	3881	3893	rVB8	65205	199754	1.60%	0.280%
40	26.029	3897	3904	3914	rVB10	68199	237845	1.90%	0.334%
41	27.786	4195	4203	4214	rVB10	94396	337186	2.69%	0.473%
42	29.995	4572	4579	4585	rBV10	71044	197711	1.58%	0.277%

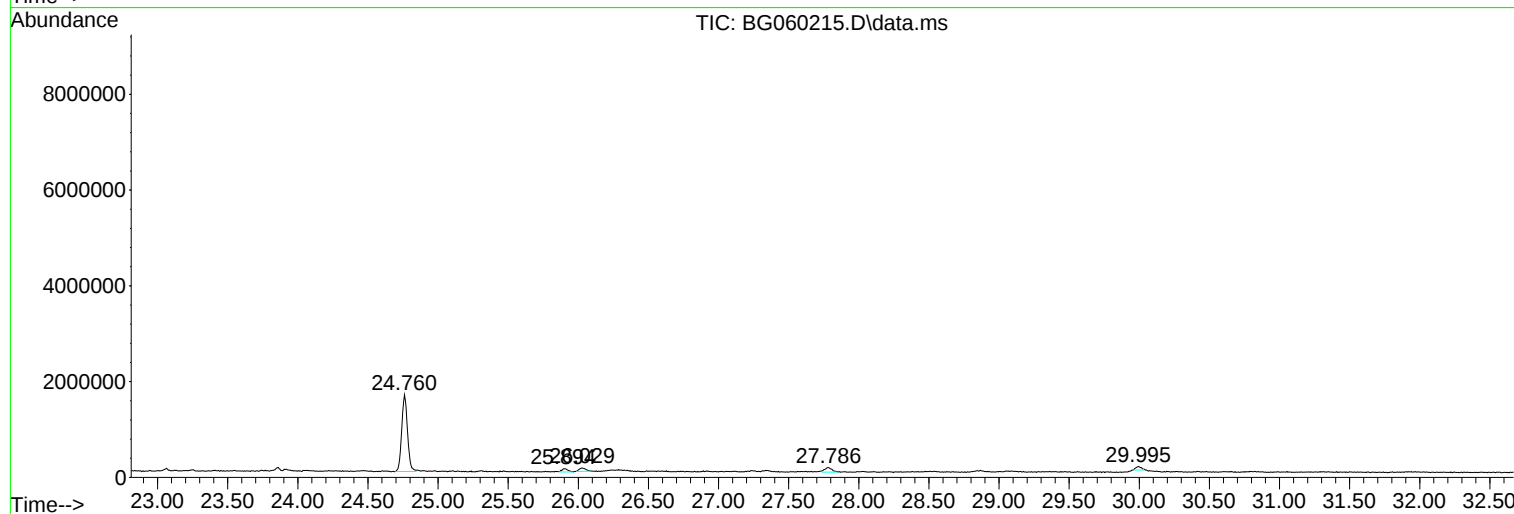
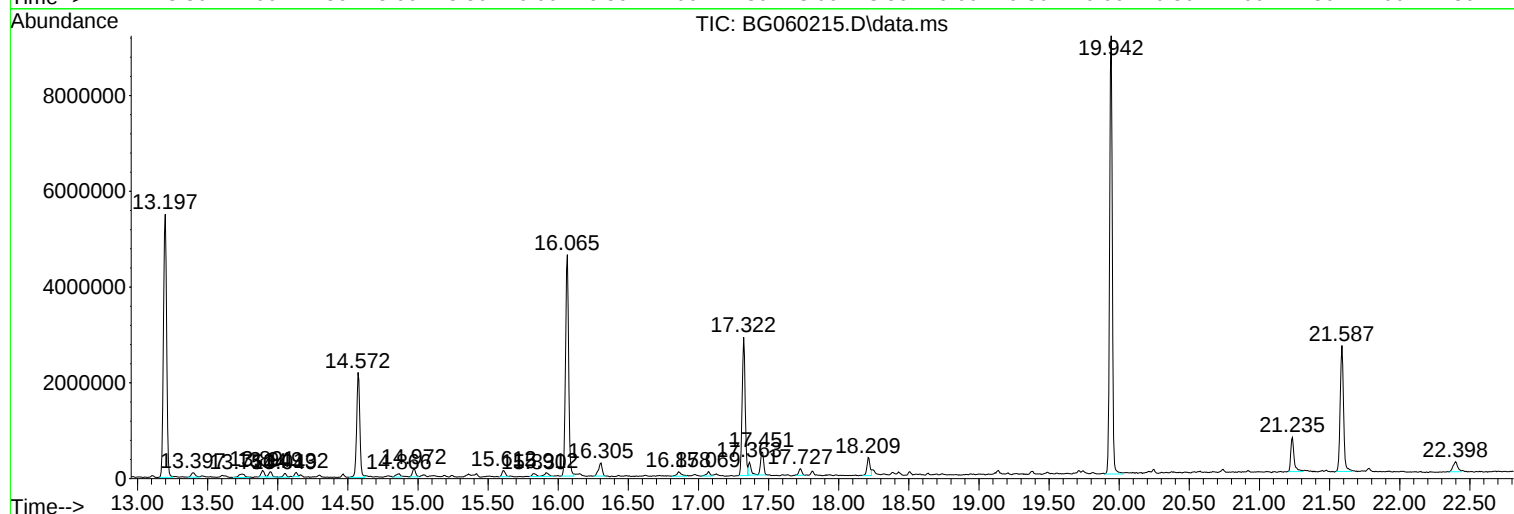
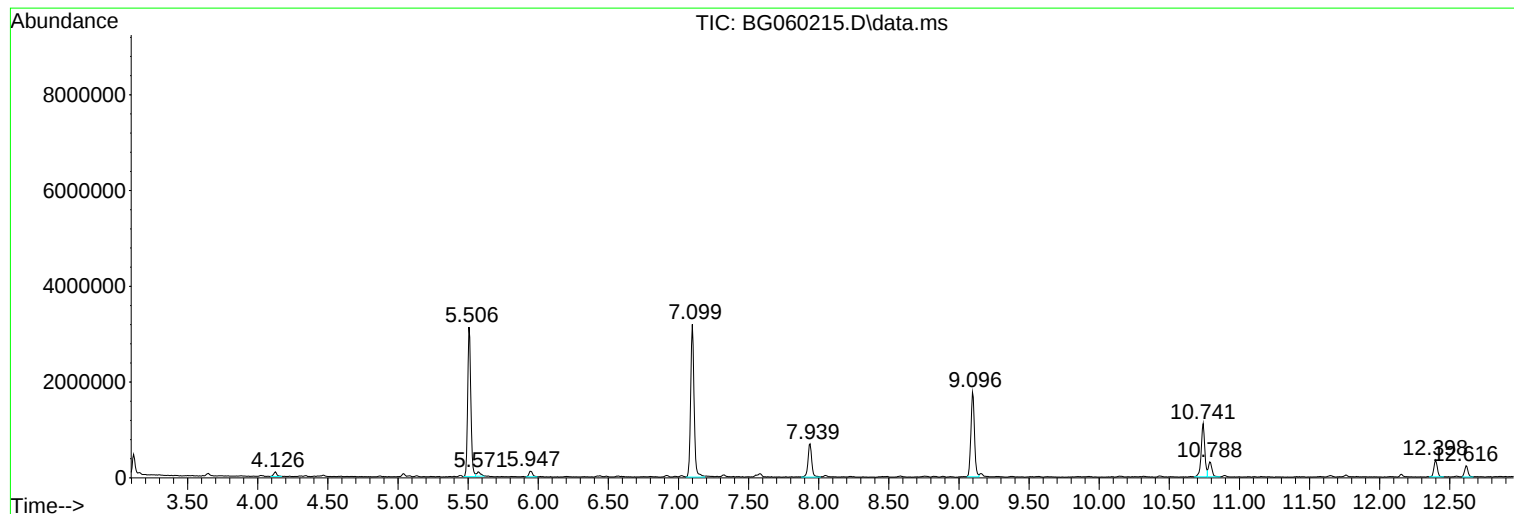
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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BNA_G
ClientSampleId :
GHL-SS-07-0-2

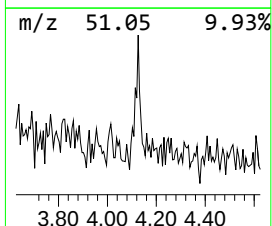
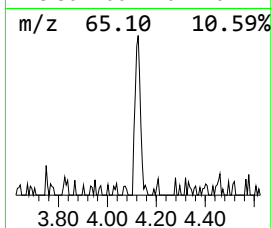
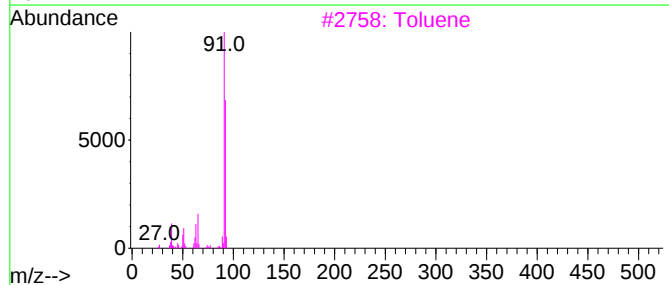
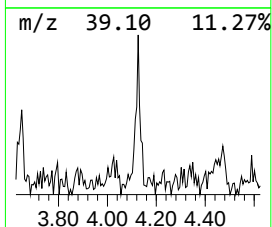
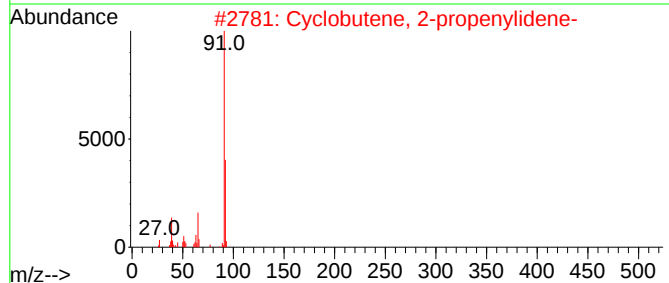
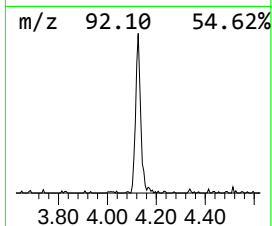
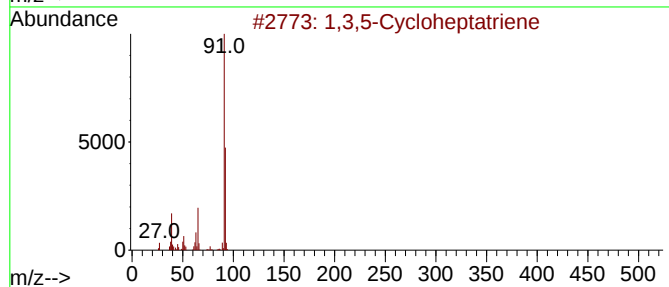
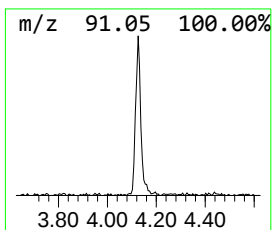
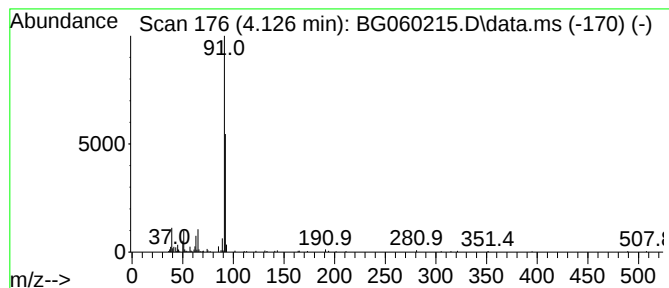
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.126	2.37 ng	150992	1,4-Dichlorobenzene-d4	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	80
2			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	80
3			Toluene	92	C7H8	000108-88-3	74
4			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	58
5			Benzeneacetamide	135	C8H9NO	000103-81-1	53



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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-0-2

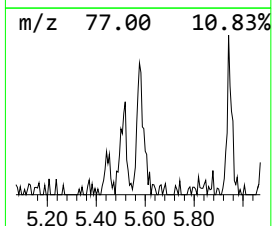
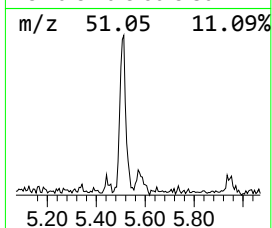
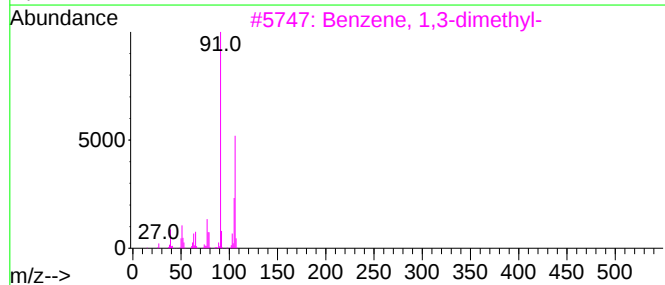
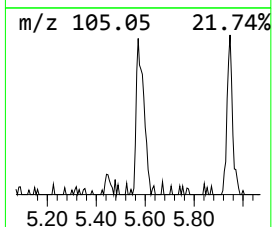
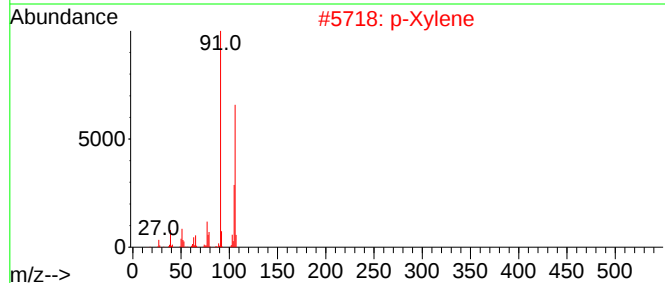
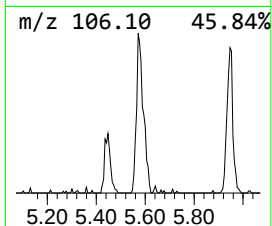
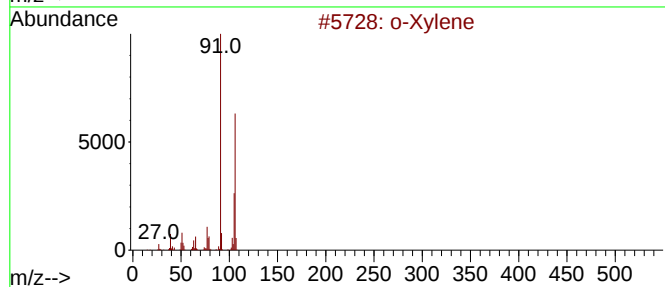
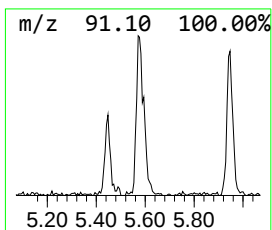
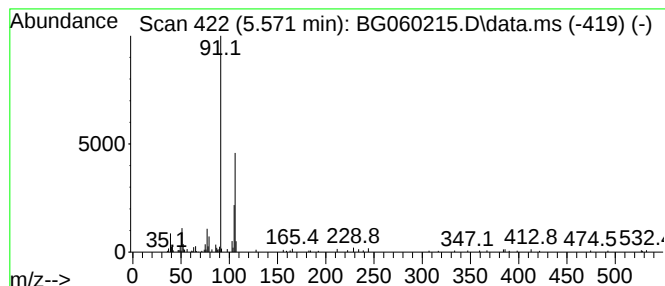
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 o-Xylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.571	2.86 ng	182198	1,4-Dichlorobenzene-d4	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Xylene	106	C8H10	000095-47-6	81
2			p-Xylene	106	C8H10	000106-42-3	74
3			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	74
4			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	64
5			Ethylbenzene	106	C8H10	000100-41-4	50



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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GHL-SS-07-0-2

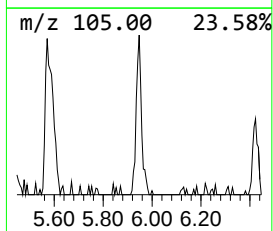
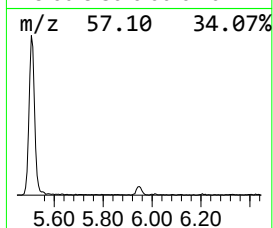
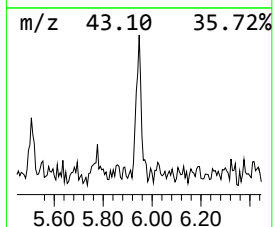
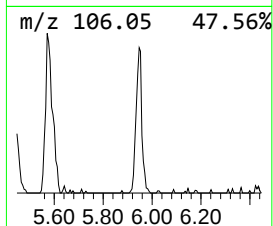
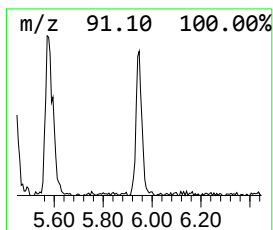
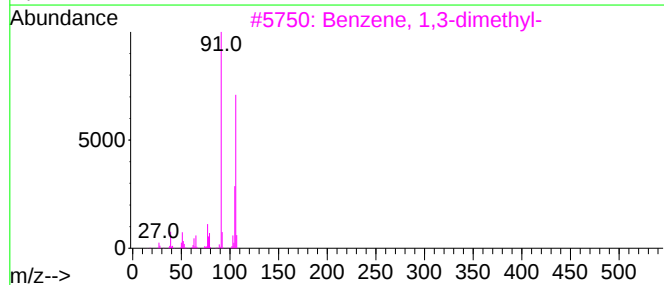
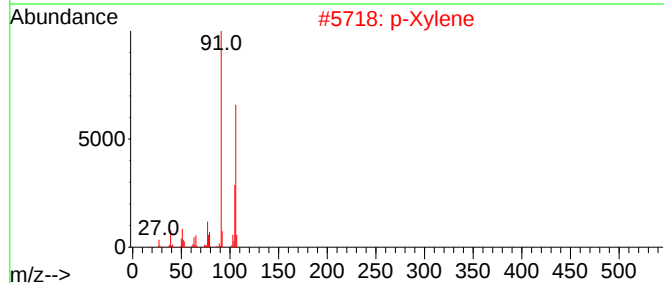
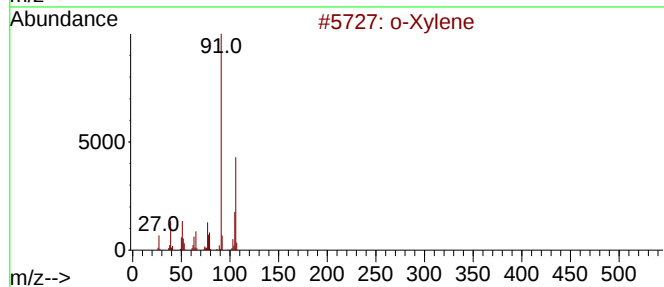
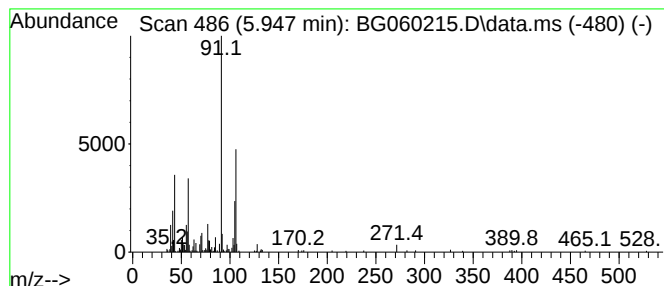
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 p-Xylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.947	3.33 ng	211984	1,4-Dichlorobenzene-d4	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Xylene	106	C8H10	000095-47-6	81
2			p-Xylene	106	C8H10	000106-42-3	81
3			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	81
4			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	64
5			Cyclopentene, 1-ethenyl-3-methyl...	106	C8H10	061142-07-2	53



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Instrument :
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ClientSampleId :
GHL-SS-07-0-2

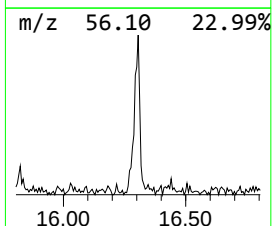
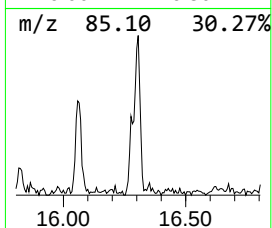
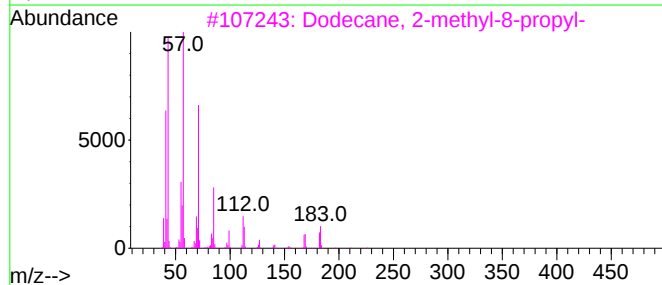
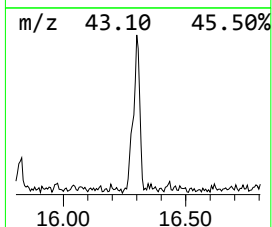
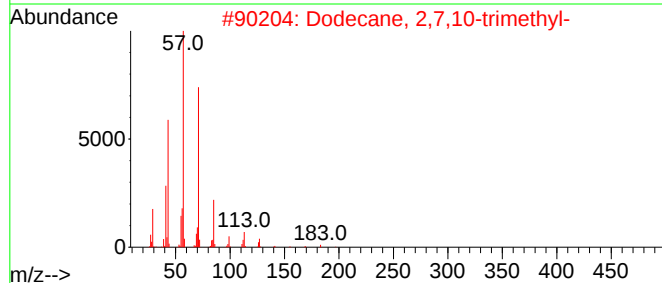
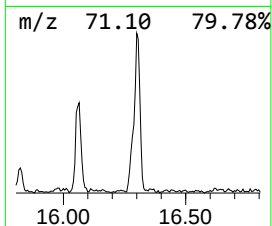
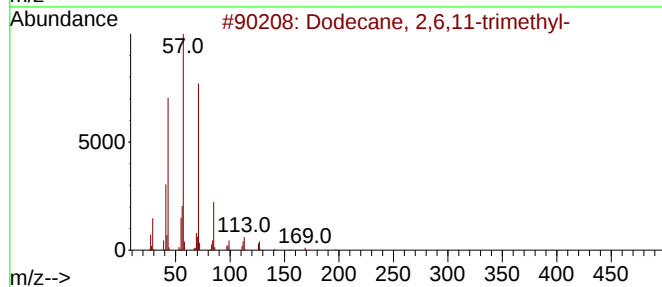
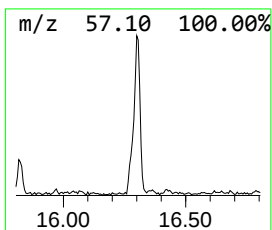
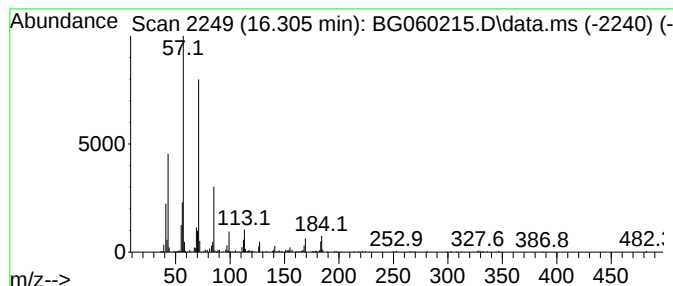
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecane, 2,6,11-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.305	2.39 ng	513500	Phenanthrene-d10	17.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
2			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
3			Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	83
4			Tridecane	184	C13H28	000629-50-5	76
5			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64



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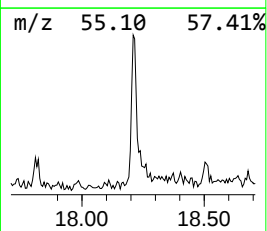
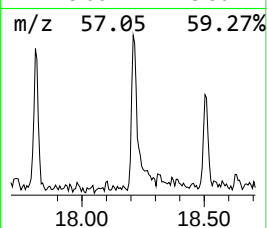
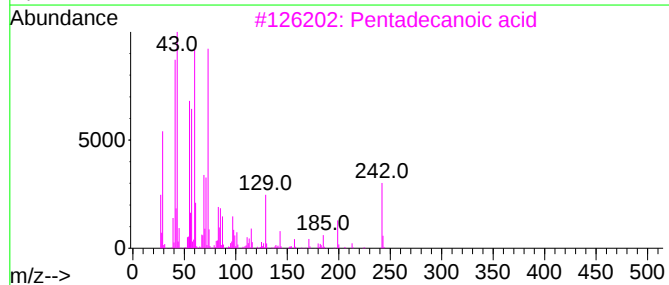
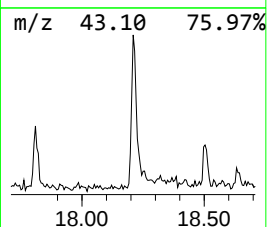
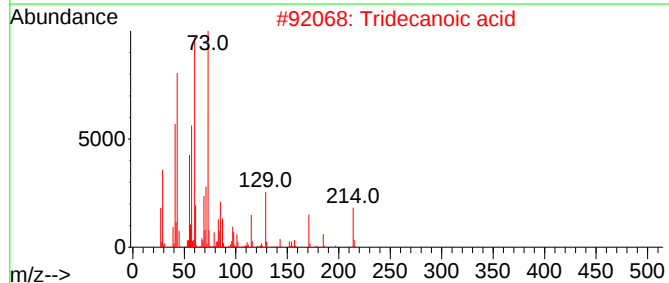
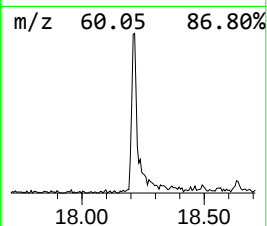
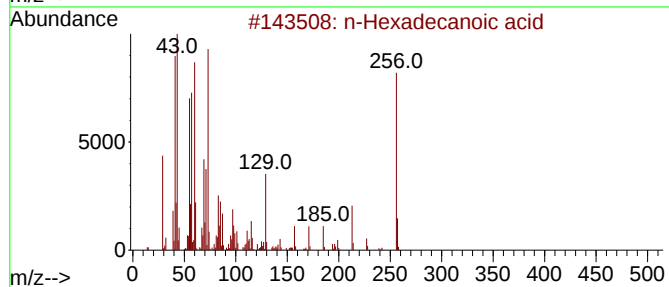
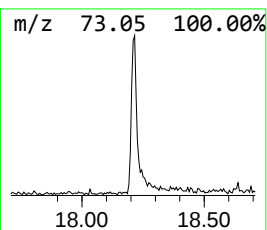
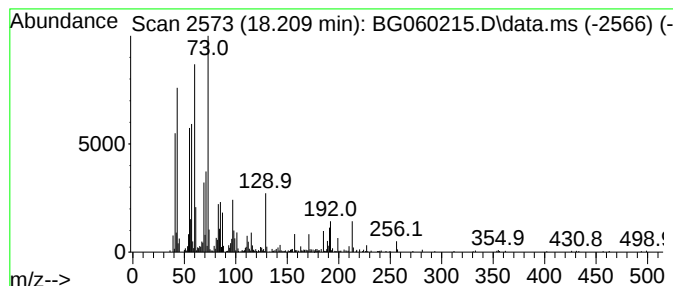
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	2.75 ng	591629	Phenanthrene-d10	17.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	76
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Undecanoic acid	186	C11H22O2	000112-37-8	64
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060215.D
Acq On : 3 Jan 2024 5:58
Operator : MA/JU
Sample : 05899-19
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-0-2

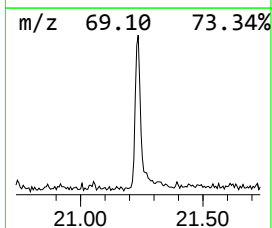
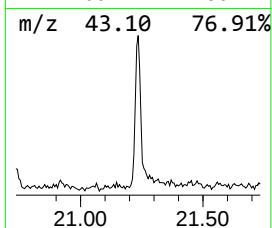
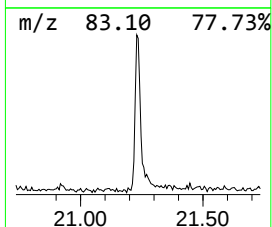
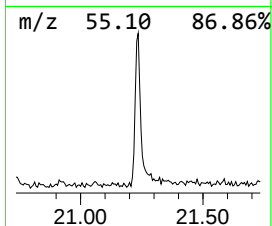
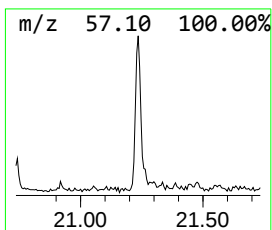
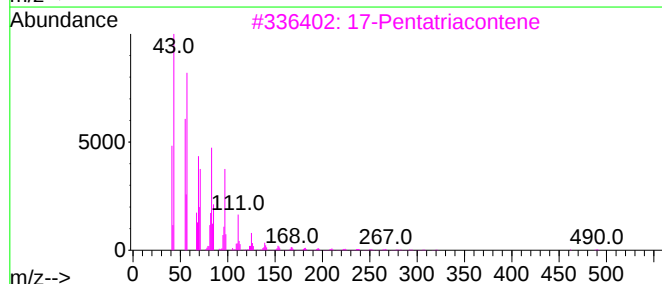
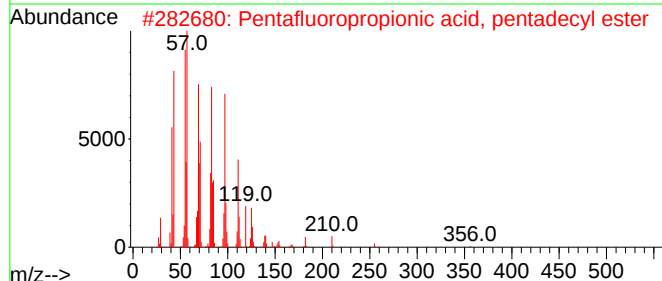
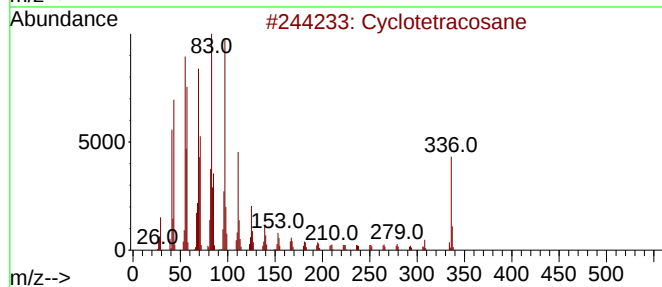
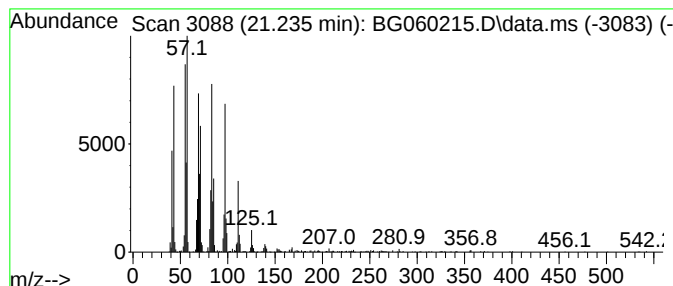
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclotetracosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.235	5.42 ng	1176510	Chrysene-d12	21.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	91
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3			17-Pentatriacontene	491	C35H70	006971-40-0	91
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5			1-Octadecanol	270	C18H38O	000112-92-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060215.D
Acq On : 3 Jan 2024 5:58
Operator : MA/JU
Sample : 05899-19
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-0-2

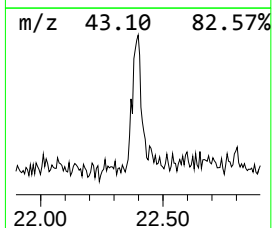
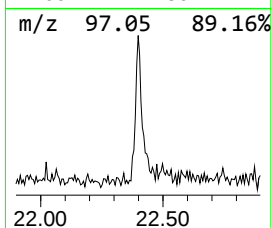
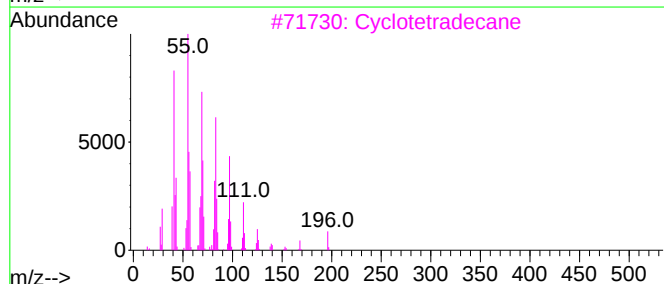
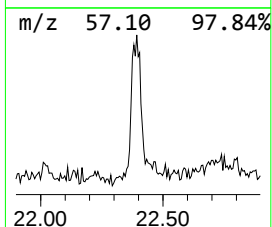
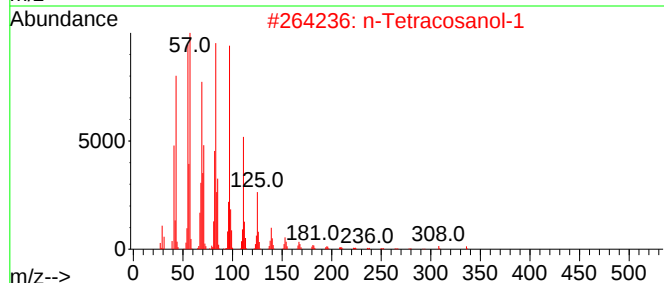
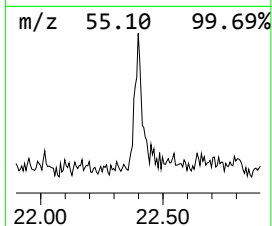
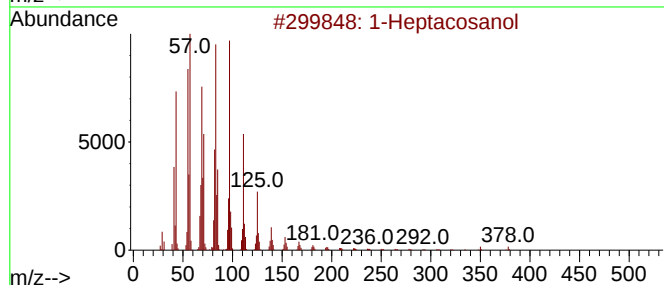
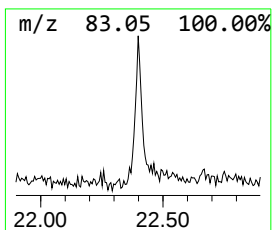
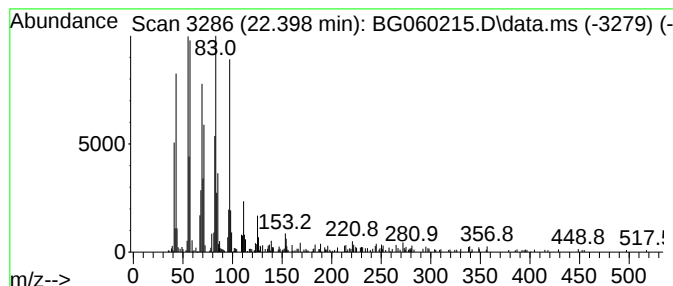
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.398	2.19 ng	474389	Chrysene-d12	21.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	91
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			Cyclotetradecane	196	C14H28	000295-17-0	90
4			Octacosanol	410	C28H58O	000557-61-9	87
5			5-Eicosene, (E)-	280	C20H40	074685-30-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060215.D
Acq On : 3 Jan 2024 5:58
Operator : MA/JU
Sample : 05899-19
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-07-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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
1,3,5-Cyclohept...	4.126	2.4	ng	150992	1	7.939	1272090	20.0
o-Xylene	5.571	2.9	ng	182198	1	7.939	1272090	20.0
p-Xylene	5.947	3.3	ng	211984	1	7.939	1272090	20.0
Dodecane, 2,6,1...	16.305	2.4	ng	513500	4	17.322	4303670	20.0
n-Hexadecanoic ...	18.209	2.8	ng	591629	4	17.322	4303670	20.0
Cyclotetracosane	21.235	5.4	ng	1176510	5	21.587	4339690	20.0
1-Heptacosanol	22.398	2.2	ng	474389	5	21.587	4339690	20.0