

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113023\
 Data File : BF136319.D
 Acq On : 30 Nov 2023 18:05
 Operator : CG\JU
 Sample : 05556-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-COMP

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_F\Methods\8270-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	11	18	rVB	455411	648099	20.15%	2.855%
2	4.440	394	400	405	rBV	84552	93047	2.89%	0.410%
3	5.051	499	504	509	rVB	286359	354045	11.01%	1.560%
4	5.445	566	571	574	rBV	2718989	2408419	74.87%	10.610%
5	6.439	734	740	743	rBV	2595424	2506837	77.93%	11.043%
6	6.804	798	802	805	rBV	997162	774607	24.08%	3.412%
7	7.363	890	897	900	rBV	1859487	1687569	52.46%	7.434%
8	8.081	1014	1019	1022	rBV	1221031	1035119	32.18%	4.560%
9	9.157	1197	1202	1205	rBV	3710702	3216940	100.00%	14.172%
10	9.833	1311	1317	1321	rBV	1109169	1030531	32.03%	4.540%
11	9.869	1321	1323	1327	rVB	40109	37232	1.16%	0.164%
12	10.627	1448	1452	1463	rBV	1106088	1029349	32.00%	4.535%
13	10.751	1470	1473	1478	rVB2	42836	54918	1.71%	0.242%
14	11.198	1543	1549	1552	rBV3	52993	65896	2.05%	0.290%
15	11.327	1567	1571	1573	rBV	985094	787760	24.49%	3.470%
16	11.351	1573	1575	1578	rVV	320854	242473	7.54%	1.068%
17	11.398	1579	1583	1587	rVB	58869	68839	2.14%	0.303%
18	11.833	1654	1657	1659	rBV	40799	37472	1.16%	0.165%
19	11.863	1659	1662	1666	rVV2	114515	110774	3.44%	0.488%
20	11.939	1672	1675	1678	rBV	54786	58328	1.81%	0.257%
21	12.127	1703	1707	1709	rBV2	37863	47174	1.47%	0.208%
22	12.380	1747	1750	1754	rBV	37589	38808	1.21%	0.171%
23	12.433	1754	1759	1762	rVV5	26199	47468	1.48%	0.209%
24	12.545	1774	1778	1781	rBV	521216	433749	13.48%	1.911%
25	12.774	1811	1817	1820	rBV	446339	426213	13.25%	1.878%
26	12.927	1839	1843	1846	rBV	2337402	2161443	67.19%	9.522%
27	12.998	1850	1855	1858	rBV2	33105	49230	1.53%	0.217%
28	13.104	1871	1873	1876	rVB	54244	46812	1.46%	0.206%
29	13.168	1880	1884	1887	rBV3	49551	53541	1.66%	0.236%
30	13.210	1887	1891	1894	rBV2	56198	64013	1.99%	0.282%
31	13.510	1939	1942	1945	rBV	40908	37902	1.18%	0.167%
32	13.615	1957	1960	1965	rVB	38925	49060	1.53%	0.216%
33	13.721	1975	1978	1981	rBV3	37106	48518	1.51%	0.214%
34	13.892	2001	2007	2014	rBV10	44092	142222	4.42%	0.627%
35	13.980	2017	2022	2025	rVV2	894534	965138	30.00%	4.252%
36	14.004	2025	2026	2029	rVB	206586	132008	4.10%	0.582%

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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_F\Methods\8270-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.368	2086	2088	2091	rVB	50957	47704	1.48%	0.210%
38	14.404	2091	2094	2097	rVB2	37053	35455	1.10%	0.156%
39	14.468	2102	2105	2107	rVV2	49227	46403	1.44%	0.204%
40	14.857	2168	2171	2177	rVB2	43690	56700	1.76%	0.250%
41	15.027	2196	2200	2203	rBV	198763	284989	8.86%	1.255%
42	15.133	2215	2218	2221	rVB3	63543	77093	2.40%	0.340%
43	15.333	2249	2252	2259	rVB	118163	144488	4.49%	0.637%
44	15.398	2259	2263	2269	rBV	149310	183055	5.69%	0.806%
45	15.462	2270	2274	2278	rBV	546581	655686	20.38%	2.888%
46	16.956	2525	2528	2540	rVB2	53076	117526	3.65%	0.518%
47	17.409	2603	2605	2612	rVB2	35164	59355	1.85%	0.261%

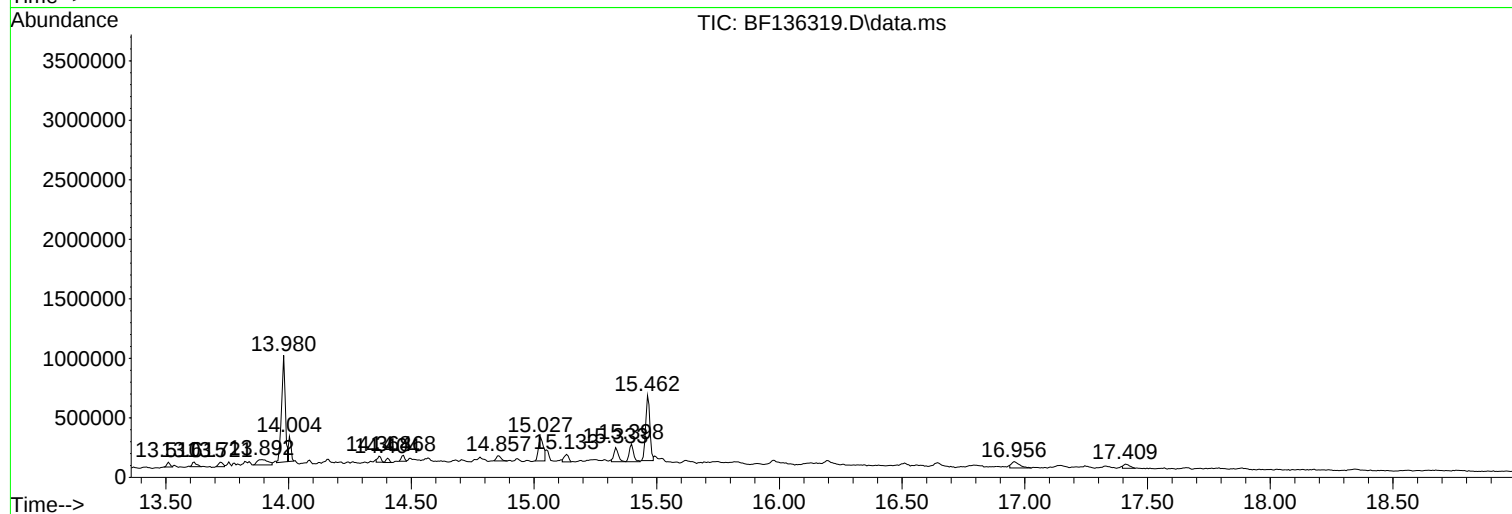
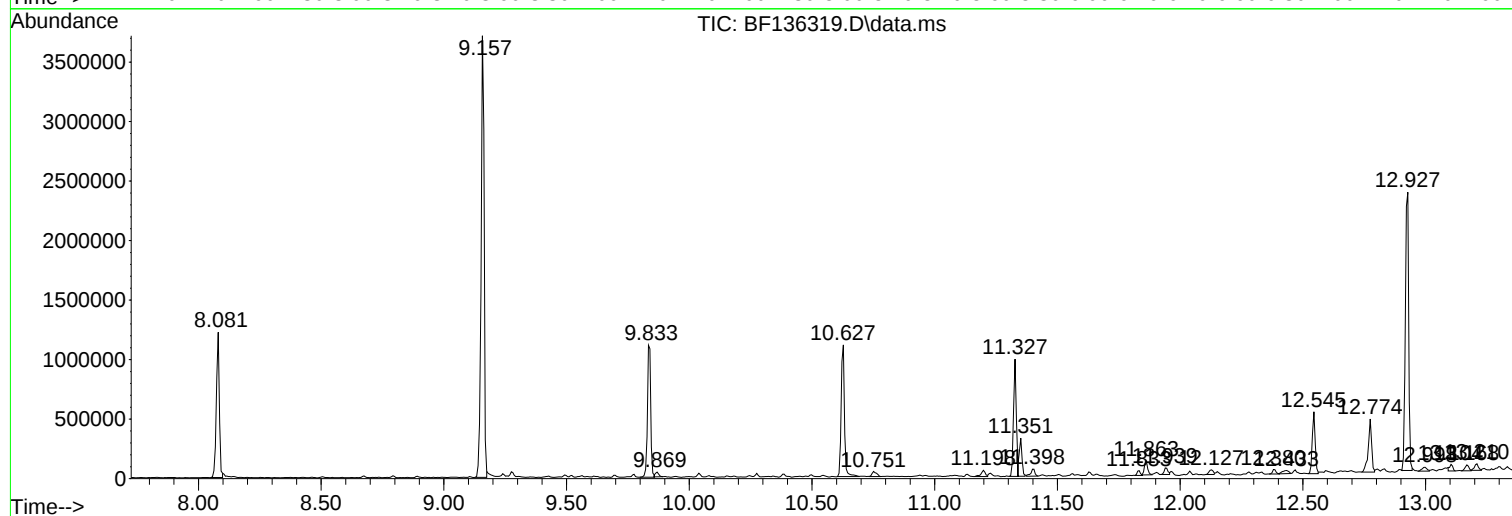
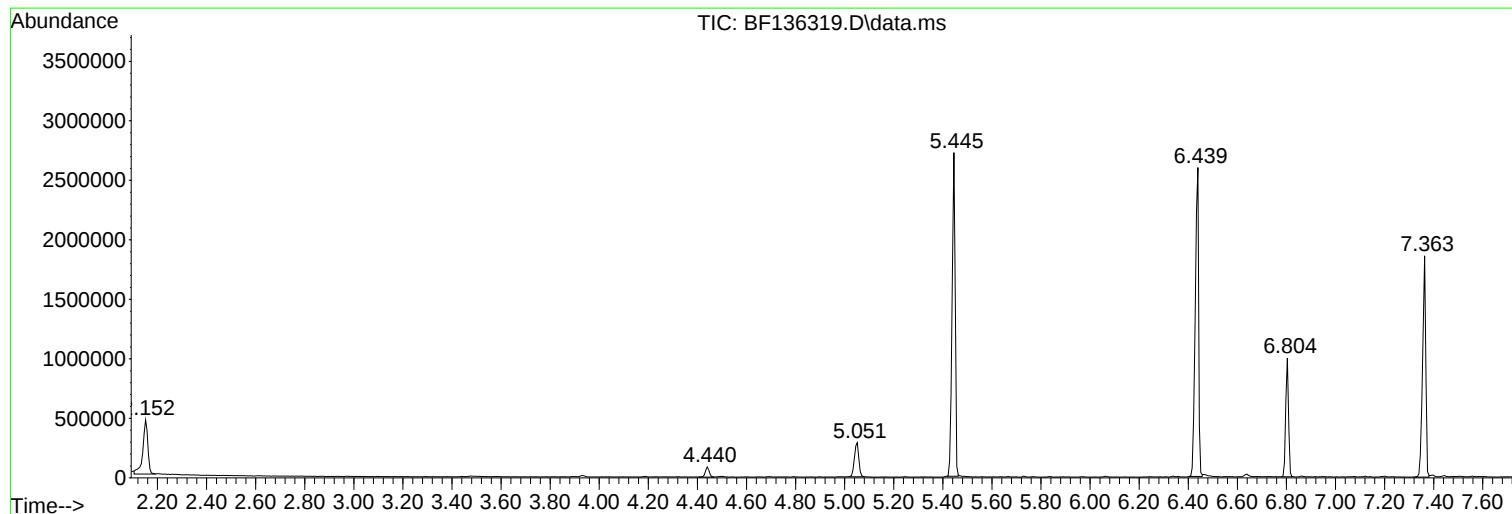
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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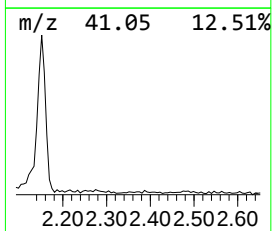
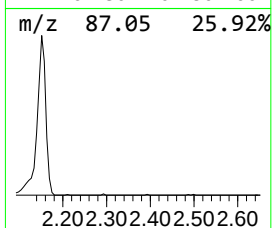
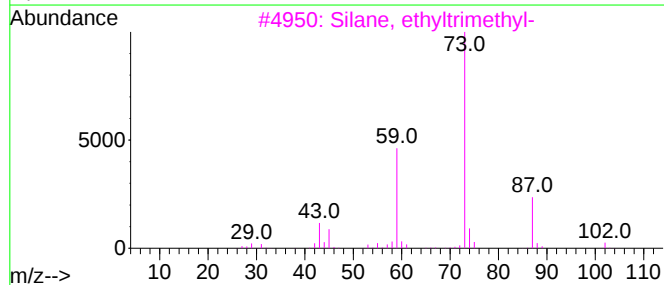
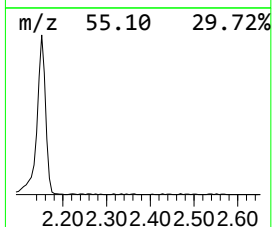
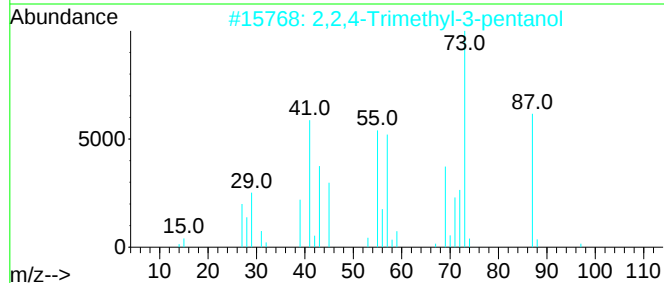
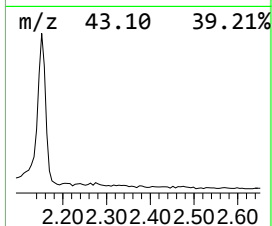
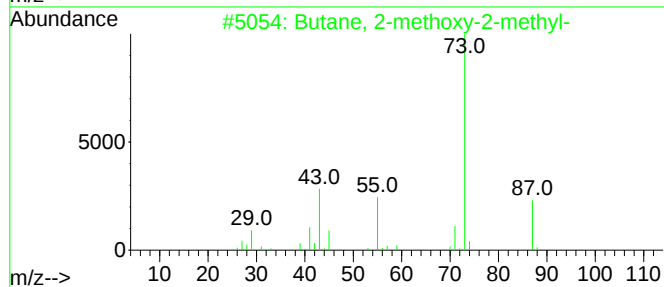
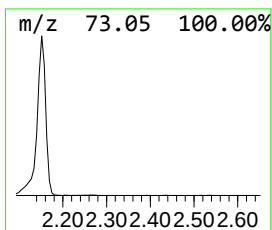
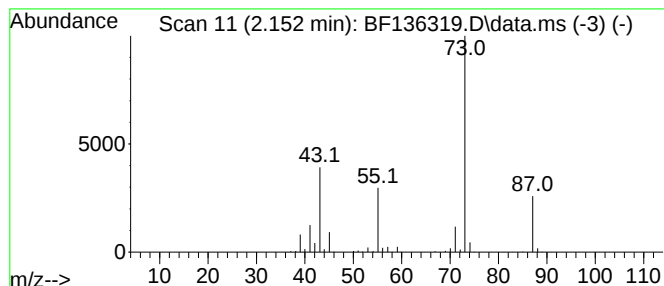
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	16.73 ng	648099	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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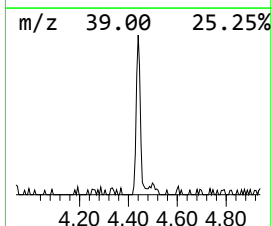
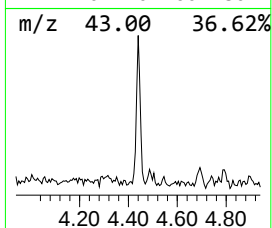
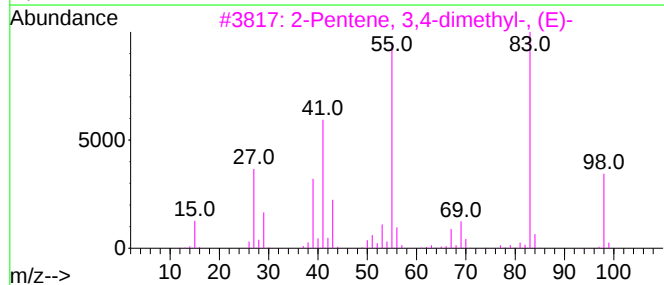
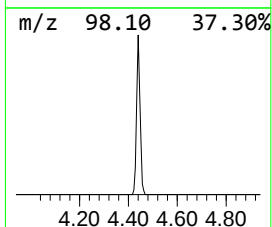
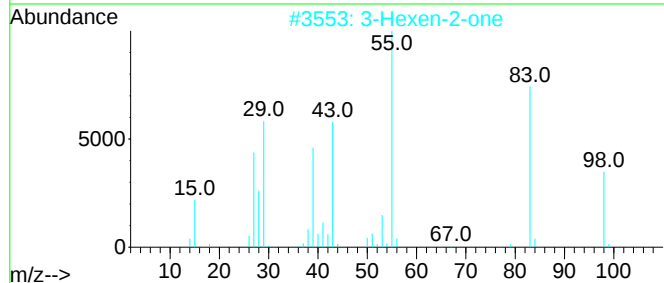
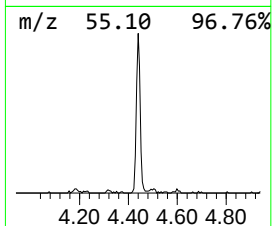
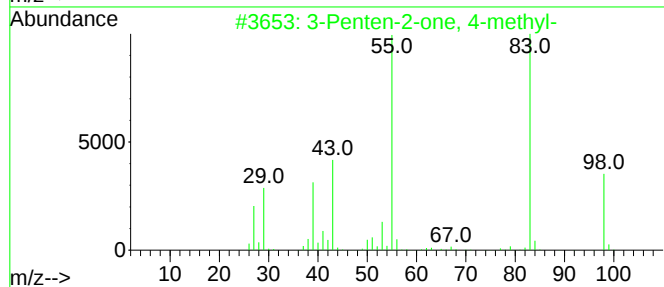
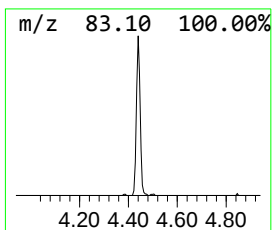
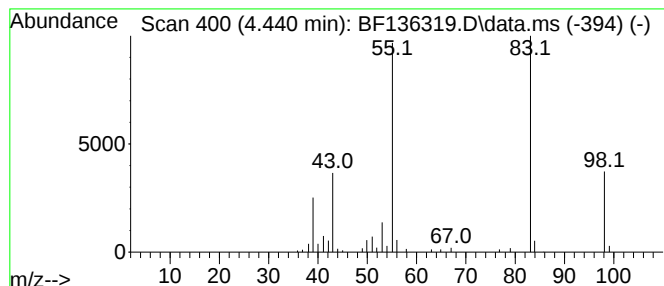
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.440	2.40 ng	93047	1,4-Dichlorobenzene-d4	6.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		Cyclohexane, methyl-	98	C7H14	000108-87-2	72



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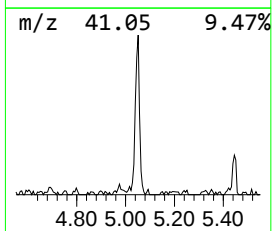
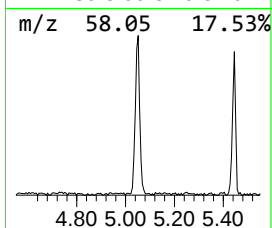
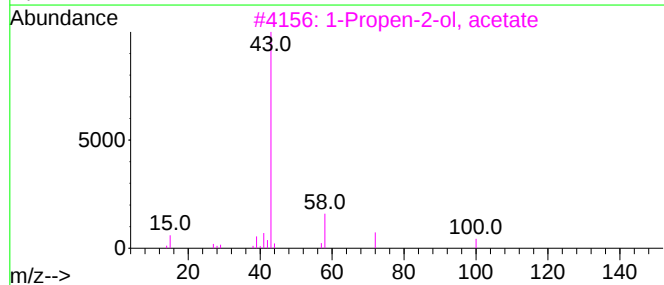
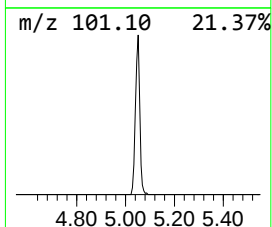
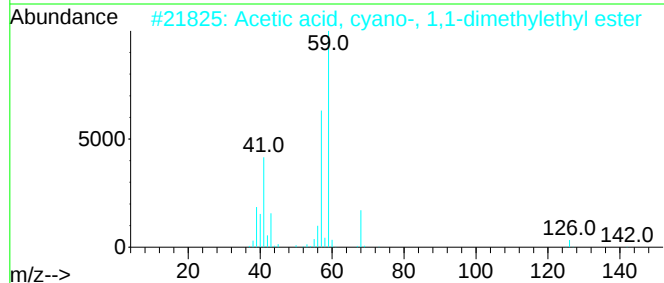
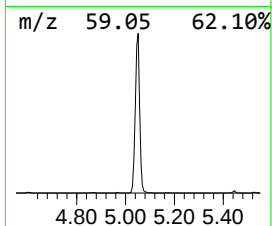
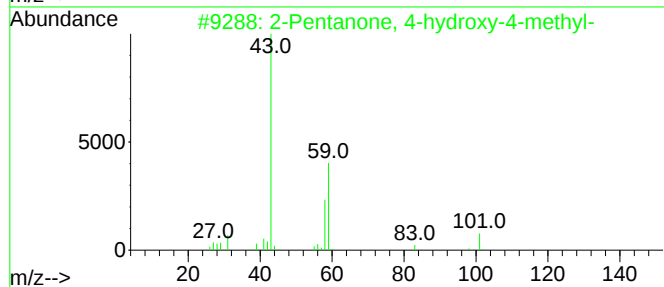
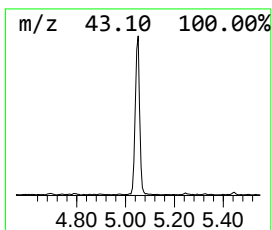
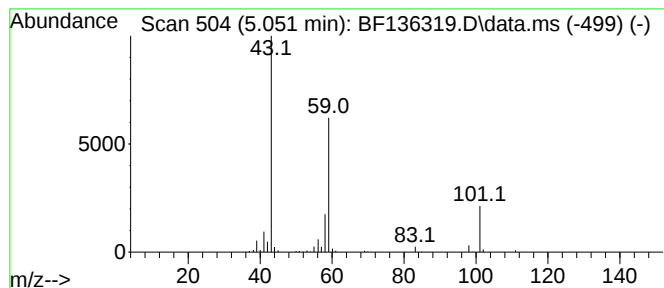
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	9.14 ng	354045	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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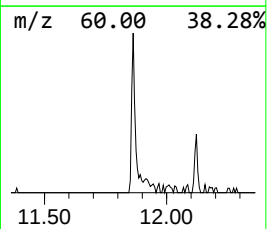
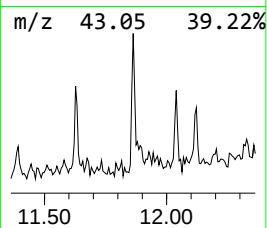
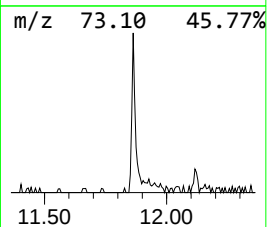
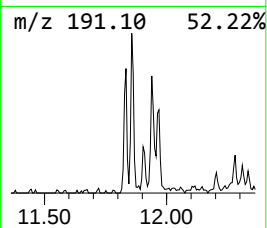
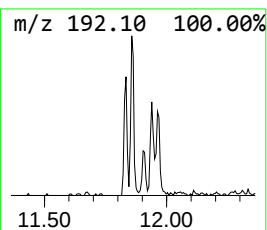
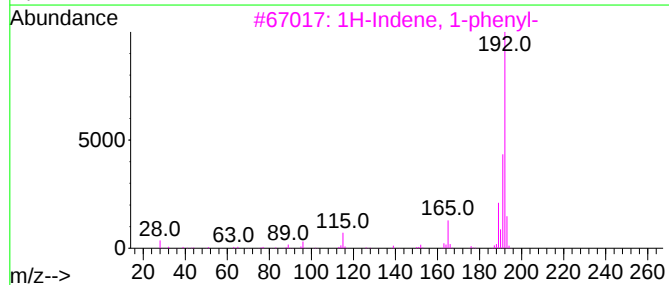
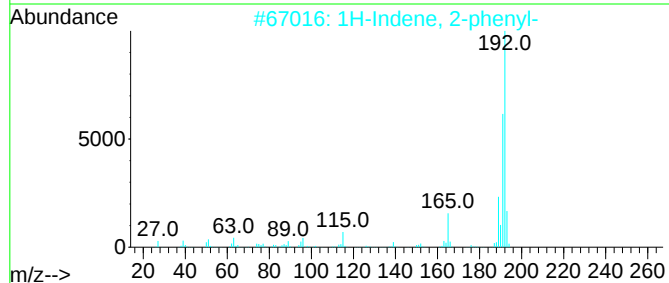
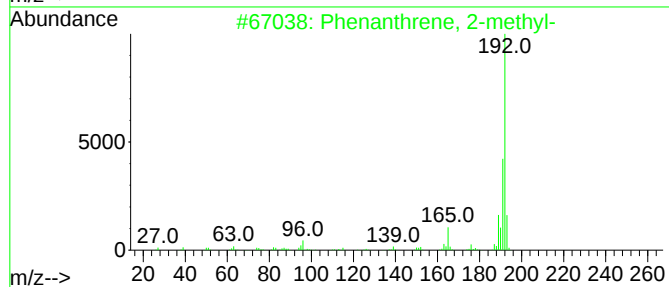
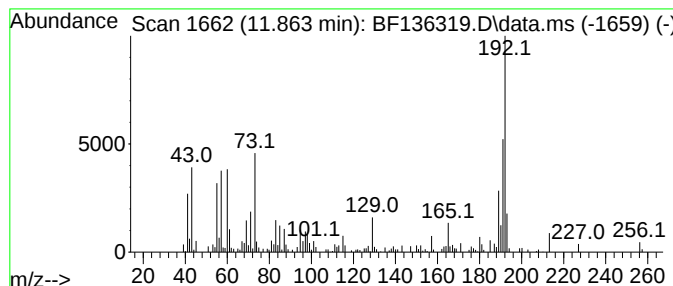
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	2.81 ng	110774	Phenanthrene-d10	11.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	92
3			1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	91
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90



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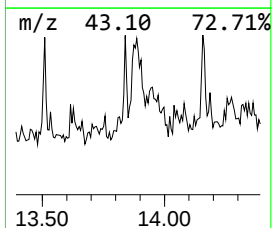
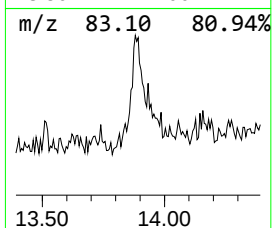
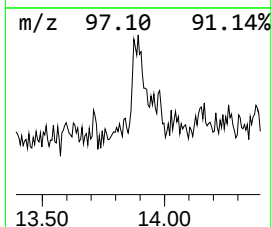
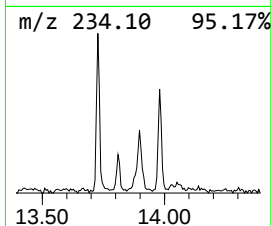
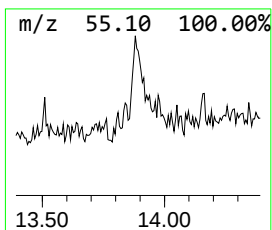
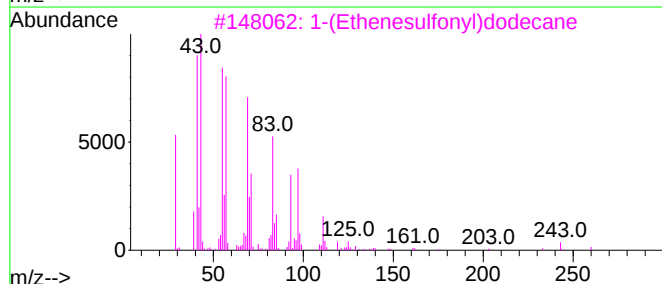
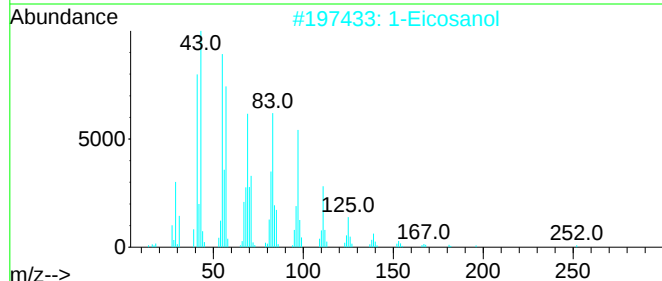
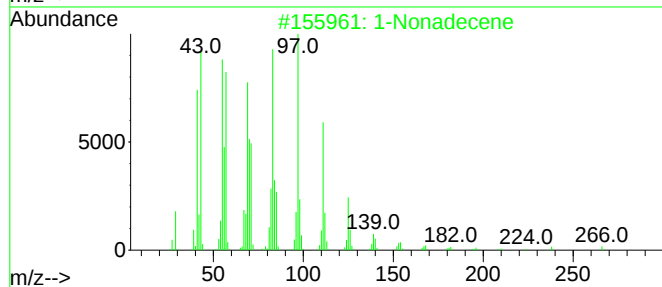
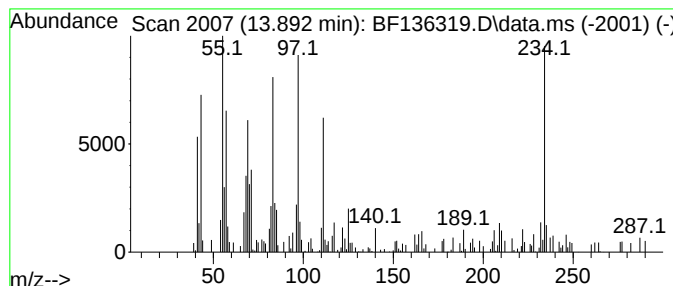
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.892 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	2.95 ng	142222	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	41
2	1-Eicosanol			298	C20H42O	000629-96-9	41
3	1-(Ethenesulfonyl)dodecane			260	C14H28O2S	030719-66-5	38
4	Cycloheptane, methyl-			112	C8H16	004126-78-7	30
5	Cyclohexane, 1-(1,5-dimethylhexy...			210	C15H30	029799-19-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113023\
Data File : BF136319.D
Acq On : 30 Nov 2023 18:05
Operator : CG\JU
Sample : 05556-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

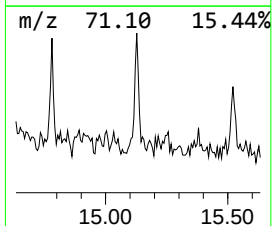
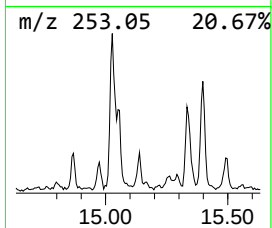
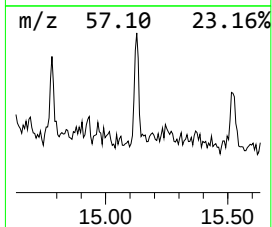
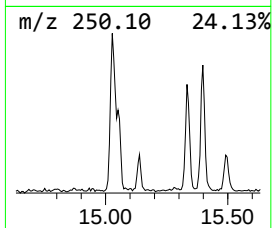
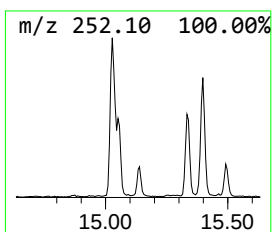
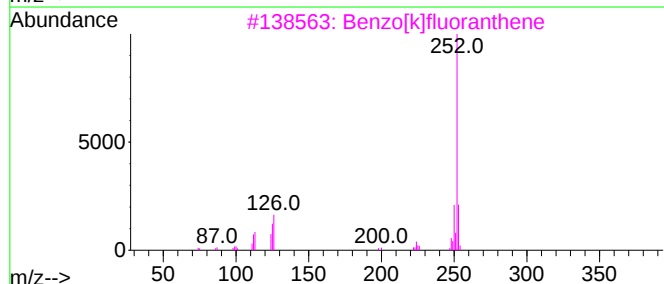
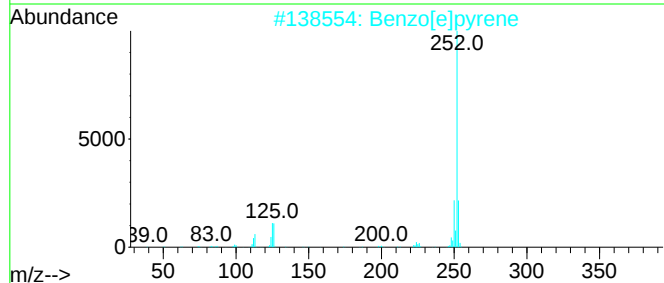
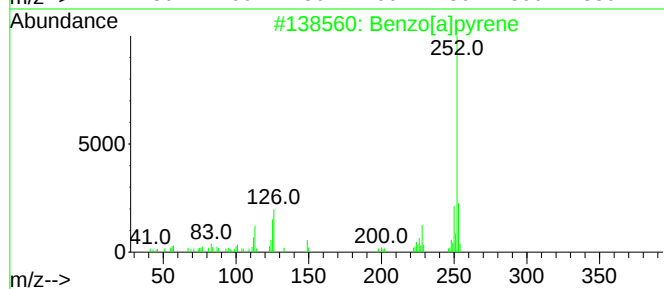
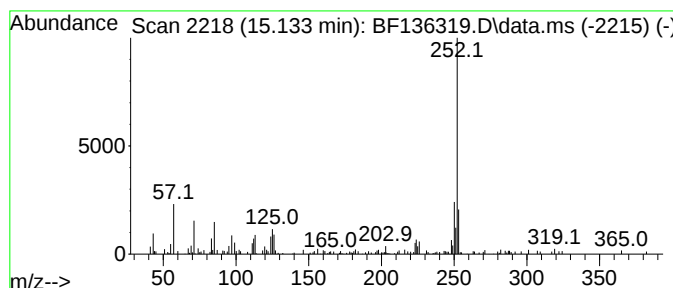
Instrument :
BNA_F
ClientSampleId :
SP-1-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.133	2.35 ng	77093	Perylene-d12	15.462	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	89
2	Benzo[e]pyrene	252	C20H12	000192-97-2	81
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
4	Perylene	252	C20H12	000198-55-0	76
5	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113023\
Data File : BF136319.D
Acq On : 30 Nov 2023 18:05
Operator : CG\JU
Sample : 05556-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-COMP

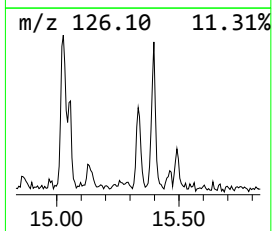
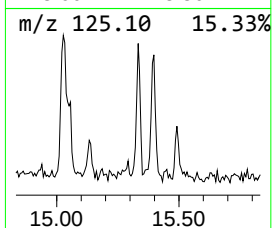
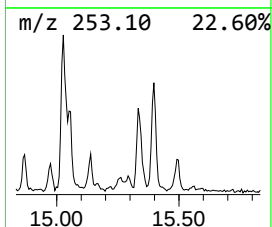
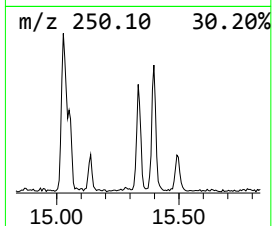
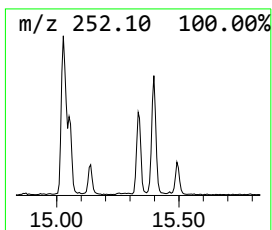
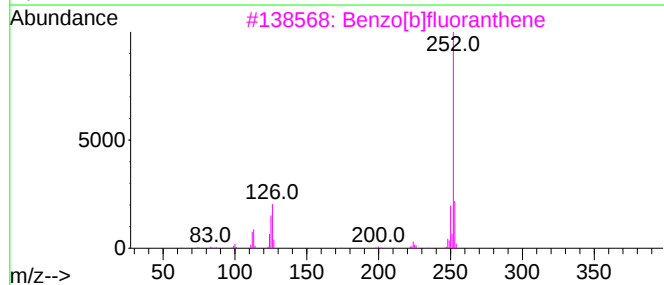
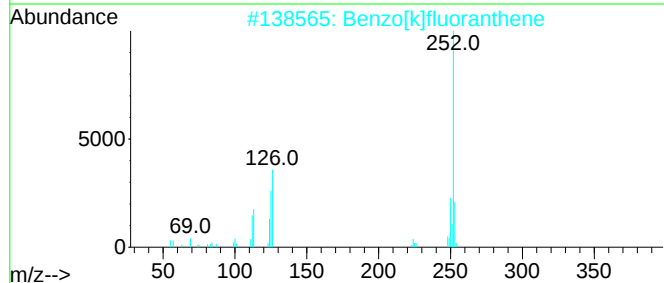
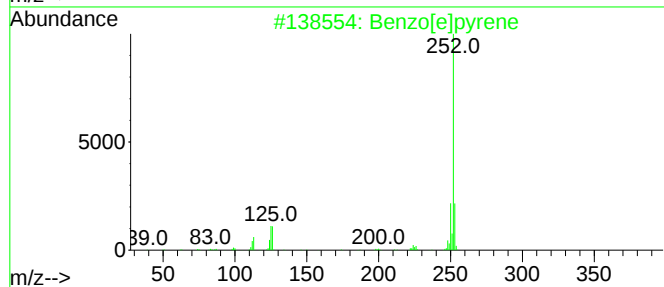
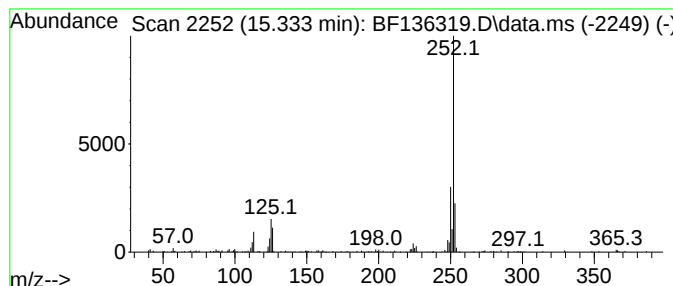
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	4.41 ng	144488	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4			Perylene	252	C20H12	000198-55-0	94
5			Benzo[a]pyrene	252	C20H12	000050-32-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113023\
Data File : BF136319.D
Acq On : 30 Nov 2023 18:05
Operator : CG\JU
Sample : 05556-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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...	2.152	16.7	ng	648099	1	6.804	774607	20.0
3-Penten-2-one,...	4.440	2.4	ng	93047	1	6.804	774607	20.0
2-Pentanone, 4-...	5.051	9.1	ng	354045	1	6.804	774607	20.0
Phenanthrene, 2...	11.863	2.8	ng	110774	4	11.327	787760	20.0
unknown13.892	13.892	3.0	ng	142222	5	13.980	965138	20.0
Benzo[e]pyrene	15.133	2.4	ng	77093	6	15.462	655686	20.0
Perylene	15.333	4.4	ng	144488	6	15.462	655686	20.0