

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
 Data File : BF137262.D
 Acq On : 02 Feb 2024 18:47
 Operator : CG\JU
 Sample : P1340-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-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_F\Methods\8270-BF013024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137262.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	13	rVB	133019	160261	8.89%	1.181%
2	5.040	498	502	510	rVB	36960	48841	2.71%	0.360%
3	5.428	564	568	583	rBV	1580183	1589610	88.23%	11.718%
4	6.422	733	737	751	rBV	1423614	1588263	88.15%	11.708%
5	6.792	796	800	809	rBV	322120	323116	17.93%	2.382%
6	7.351	890	895	908	rBV	1044735	1021687	56.71%	7.531%
7	8.069	1013	1017	1025	rBV	425161	428228	23.77%	3.157%
8	9.145	1196	1200	1203	rBV	2157537	1801700	100.00%	13.281%
9	9.822	1311	1315	1318	rBV	593985	470625	26.12%	3.469%
10	9.851	1318	1320	1326	rVB	27907	28818	1.60%	0.212%
11	10.610	1445	1449	1463	rBV	1117225	1080260	59.96%	7.963%
12	11.310	1565	1568	1571	rBV	461347	434218	24.10%	3.201%
13	11.333	1571	1572	1578	rVV	251281	200142	11.11%	1.475%
14	11.386	1578	1581	1585	rVB	42353	43530	2.42%	0.321%
15	11.816	1650	1654	1657	rBV	35388	38221	2.12%	0.282%
16	11.851	1657	1660	1665	rVV2	78443	100161	5.56%	0.738%
17	11.927	1670	1673	1675	rVV	45797	52260	2.90%	0.385%
18	11.951	1675	1677	1684	rVB	25937	27387	1.52%	0.202%
19	12.527	1772	1775	1781	rBV	338973	298226	16.55%	2.198%
20	12.757	1808	1814	1821	rBV	293209	310917	17.26%	2.292%
21	12.910	1836	1840	1847	rVV	1717148	1540432	85.50%	11.355%
22	12.980	1847	1852	1859	rVB3	23156	38207	2.12%	0.282%
23	13.092	1868	1871	1875	rVB	29250	32533	1.81%	0.240%
24	13.192	1885	1888	1891	rBV	40044	40702	2.26%	0.300%
25	13.486	1932	1938	1942	rBV7	12248	21642	1.20%	0.160%
26	13.598	1954	1957	1962	rVB	28665	31131	1.73%	0.229%
27	13.710	1971	1976	1979	rBV2	25658	36319	2.02%	0.268%
28	13.810	1990	1993	1997	rVB	23070	22409	1.24%	0.165%
29	13.963	2012	2019	2022	rBV2	506260	644817	35.79%	4.753%
30	13.986	2022	2023	2032	rVB	160019	157682	8.75%	1.162%
31	14.351	2081	2085	2089	rBV	33535	39958	2.22%	0.295%
32	14.610	2126	2129	2134	rVB3	20752	20552	1.14%	0.152%
33	14.745	2148	2152	2161	rBV4	38357	62797	3.49%	0.463%
34	14.845	2163	2169	2174	rBV5	23209	34853	1.93%	0.257%
35	15.010	2192	2197	2208	rBV	100088	219380	12.18%	1.617%
36	15.115	2212	2215	2221	rVB	33674	39010	2.17%	0.288%

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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_F\Methods\8270-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.315	2245	2249	2255	rVB	53084	67823	3.76%	0.500%
38	15.374	2255	2259	2265	rVB	72125	93182	5.17%	0.687%
39	15.439	2265	2270	2275	rBV	220125	295863	16.42%	2.181%
40	16.927	2518	2523	2532	rVB3	19493	46019	2.55%	0.339%
41	17.368	2593	2598	2606	rBV2	16143	33884	1.88%	0.250%

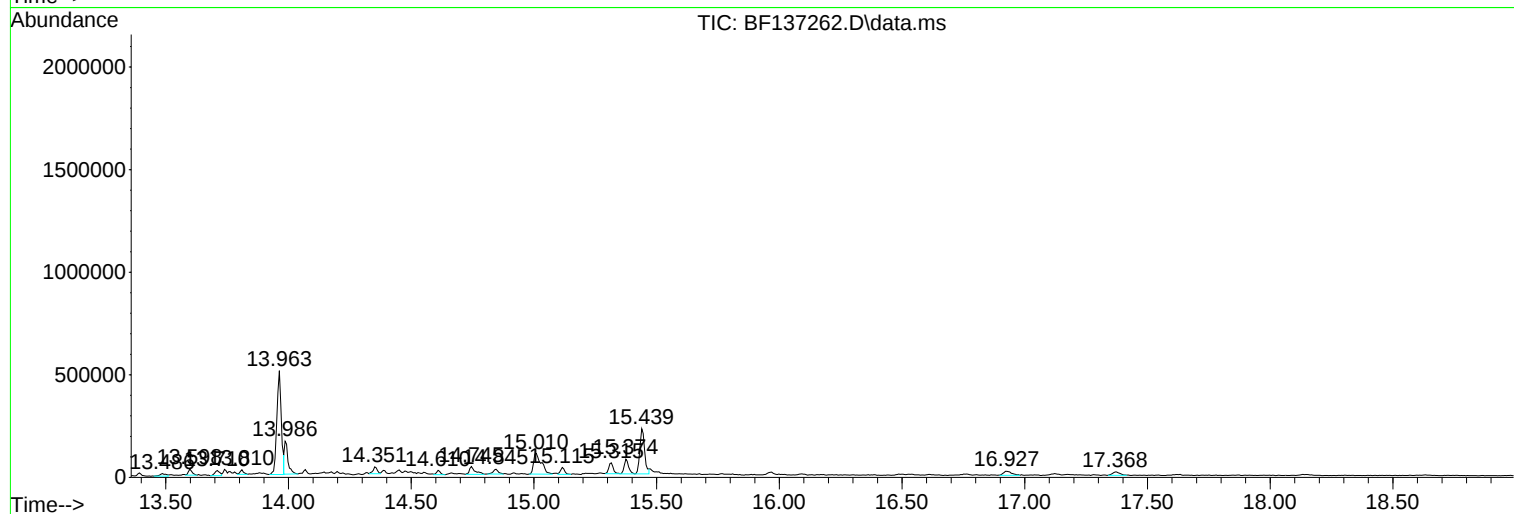
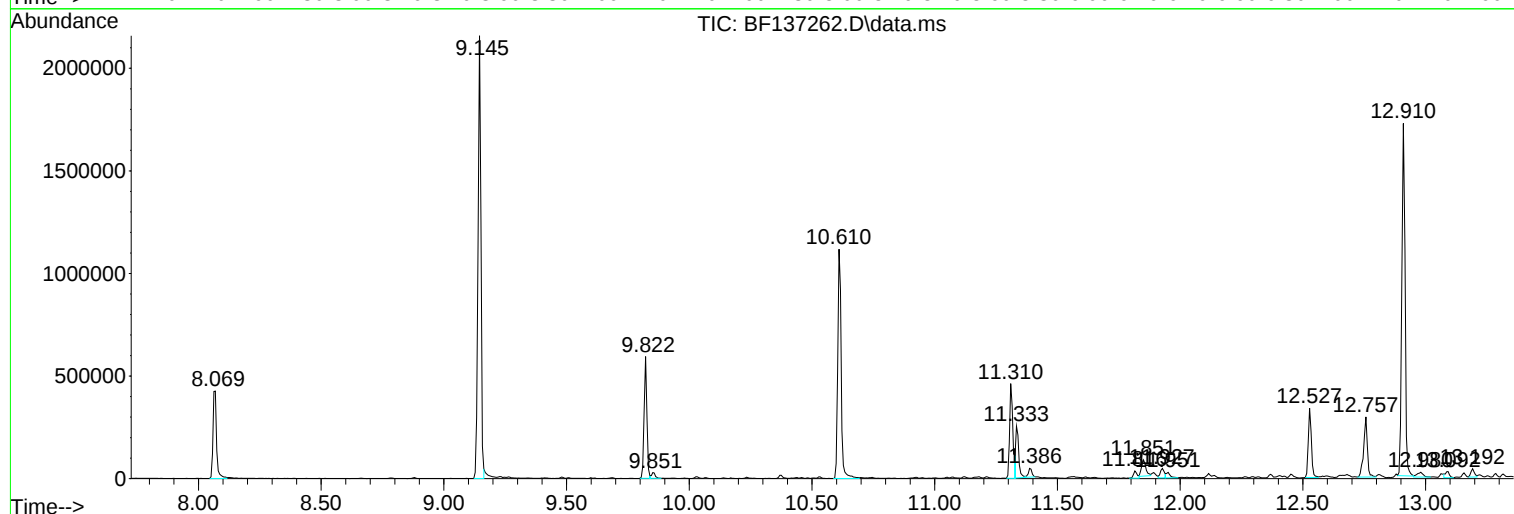
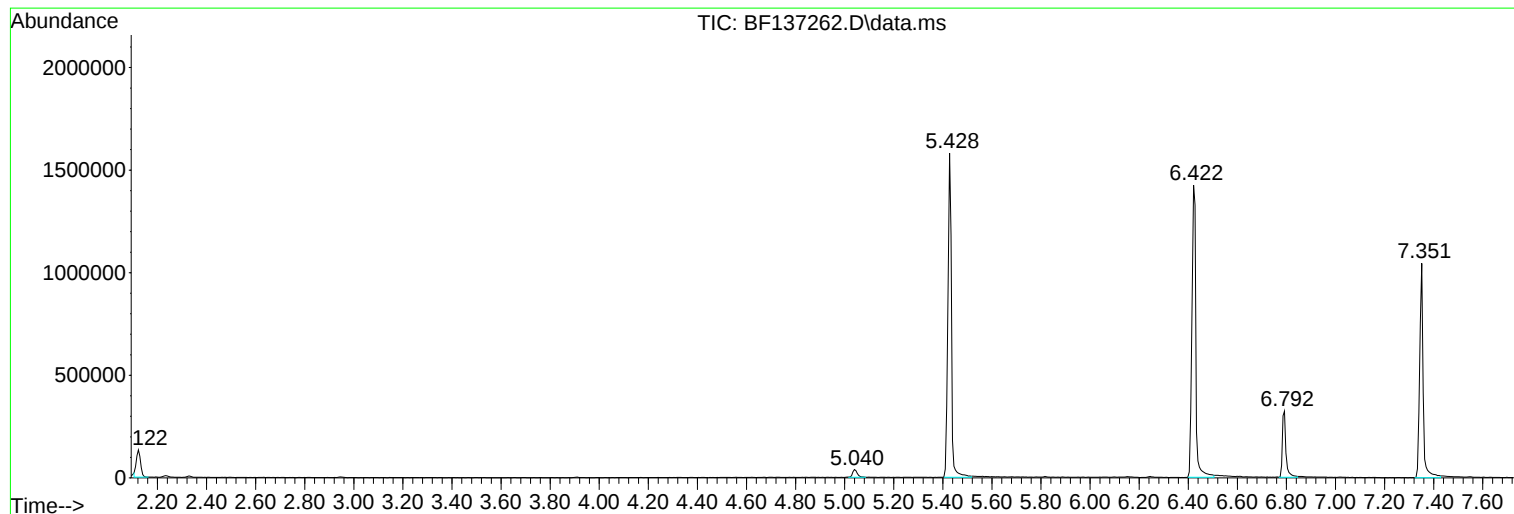
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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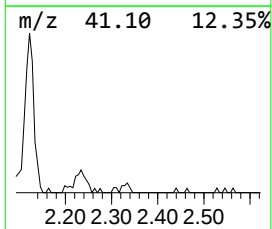
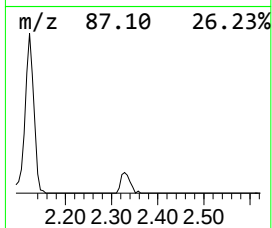
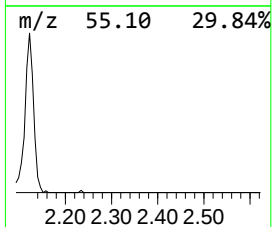
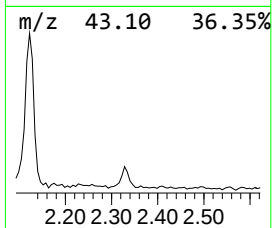
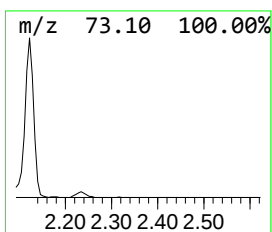
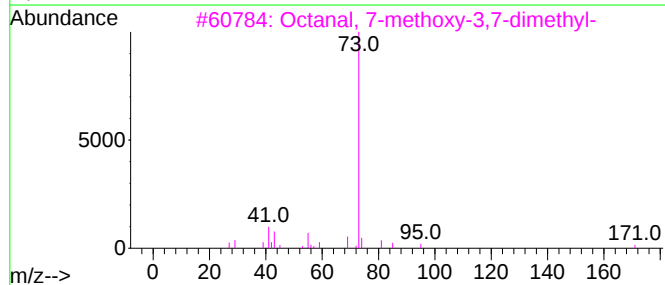
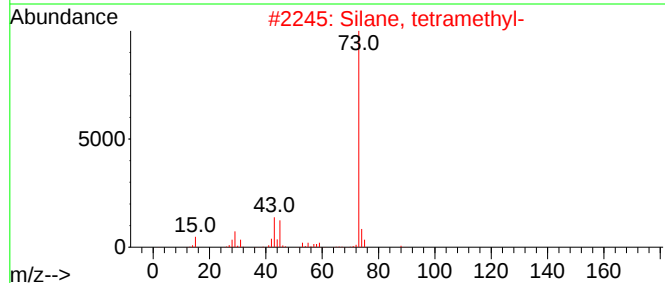
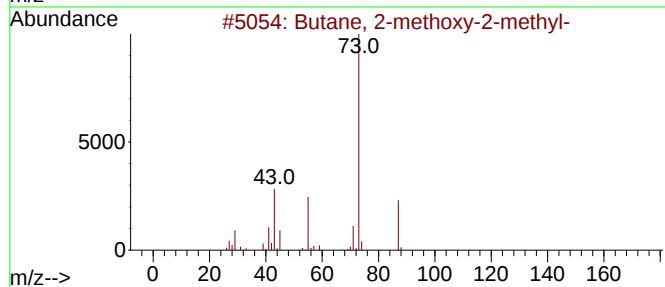
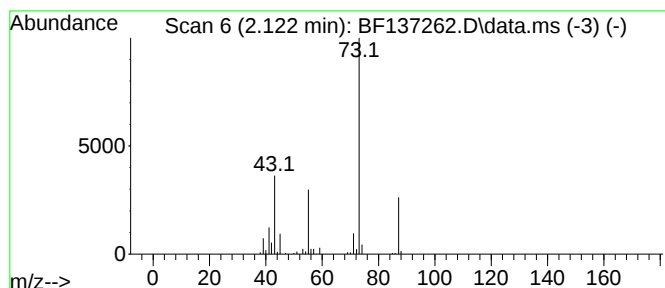
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.122	9.92 ng	160261	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10



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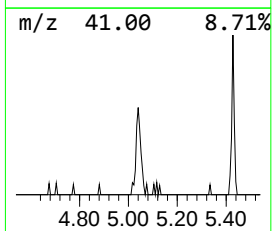
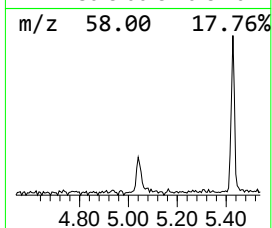
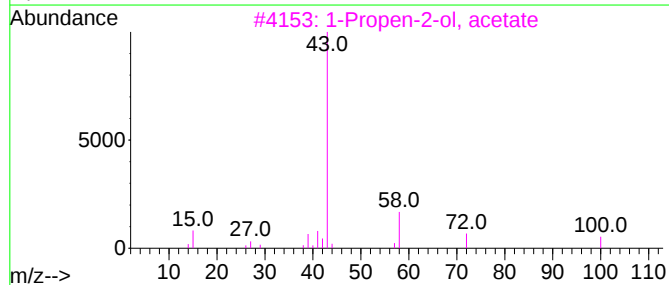
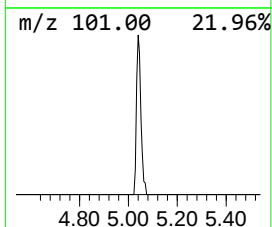
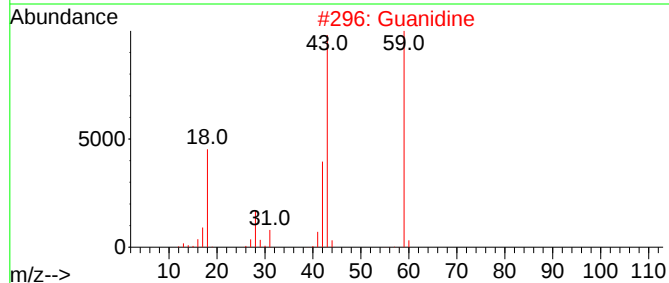
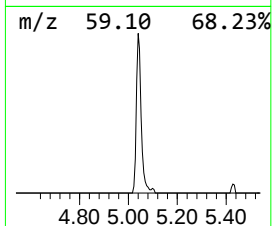
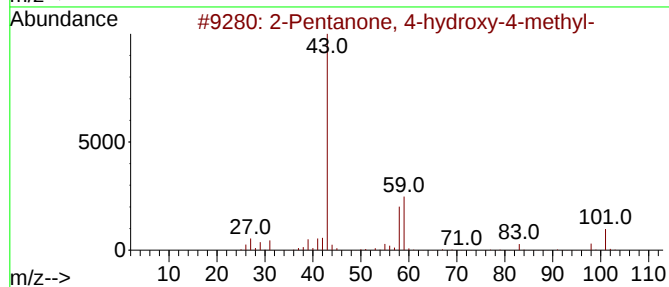
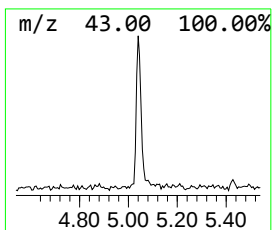
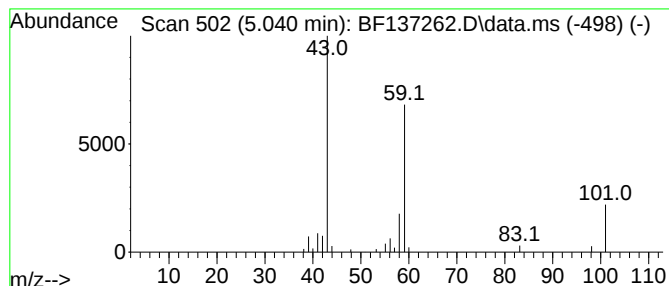
Instrument :
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ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.040	3.02 ng	48841	1,4-Dichlorobenzene-d4	6.792	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Guanidine	59	CH5N3	000113-00-8	43
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetone	58	C3H6O	000067-64-1	9
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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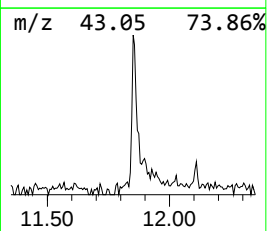
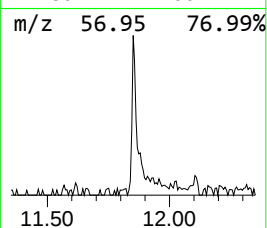
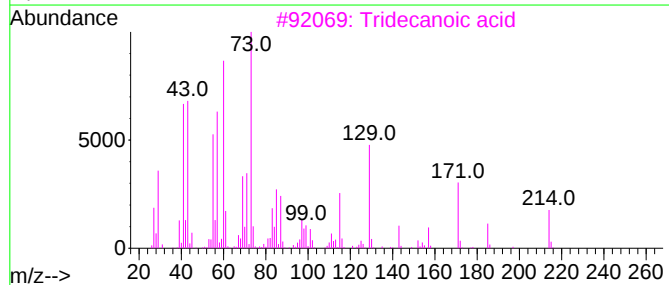
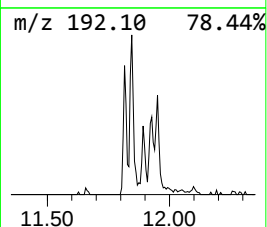
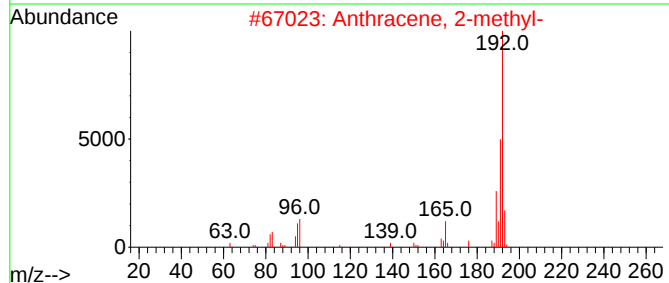
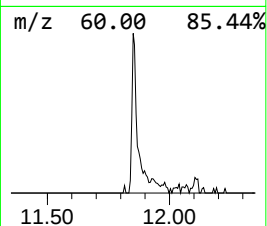
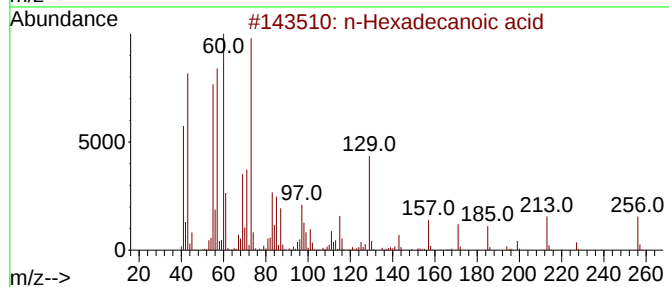
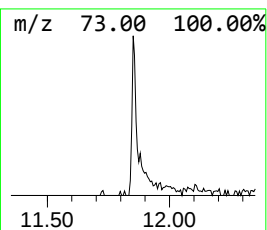
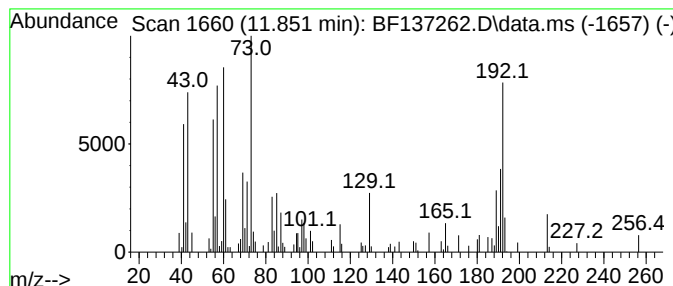
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	4.61 ng	100161	Phenanthrene-d10	11.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Anthracene, 2-methyl-	192	C15H12	000613-12-7	60
3		Tridecanoic acid	214	C13H26O2	000638-53-9	49
4		Anthracene, 9-methyl-	192	C15H12	000779-02-2	42
5		Anthracene, 1-methyl-	192	C15H12	000610-48-0	42



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Misc :
ALS Vial : 16 Sample Multiplier: 1

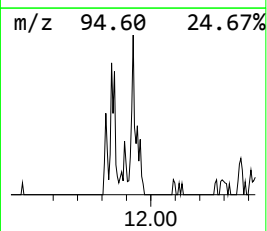
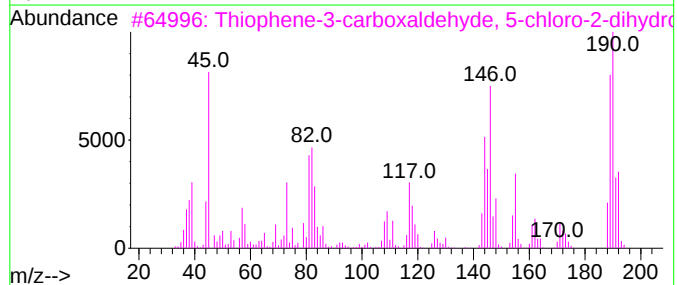
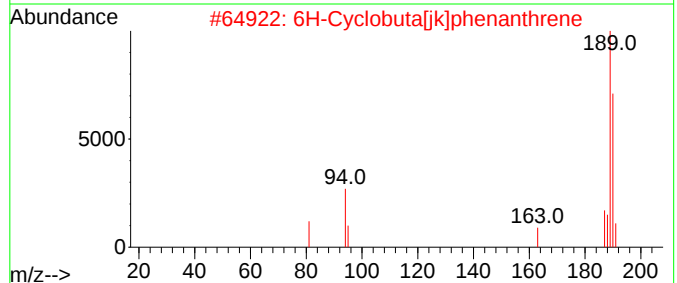
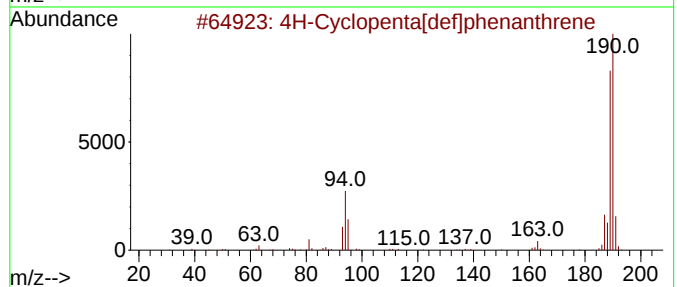
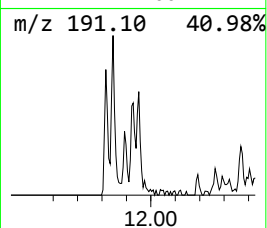
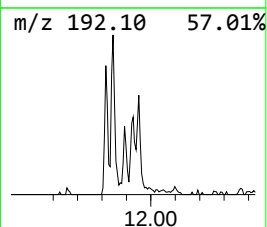
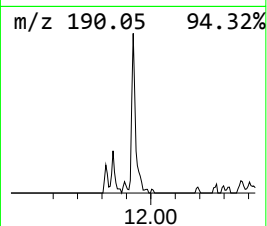
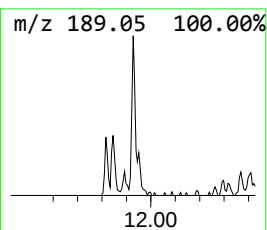
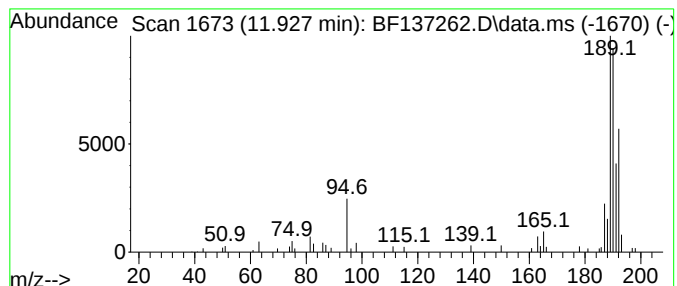
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.927	2.41 ng	52260	Phenanthrene-d10			11.310
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene		190	C15H10	083469-43-6	53
3	Thiophene-3-carboxaldehyde, 5-ch...		190	C5H4BClO3S	036155-87-0	50
4	Methyl diselenide		190	C2H6Se2	007101-31-7	38
5	4,6-Dichloro-2-ethylpyrimidin-5-...		191	C6H7Cl2N3	006237-96-3	38



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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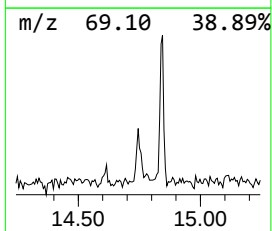
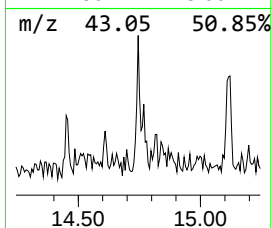
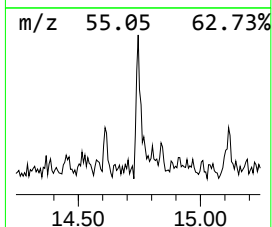
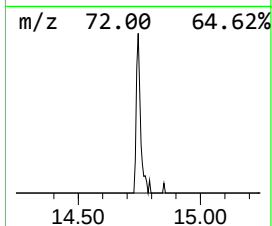
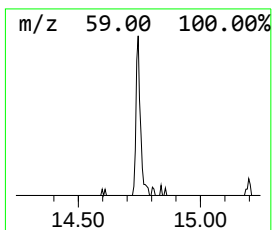
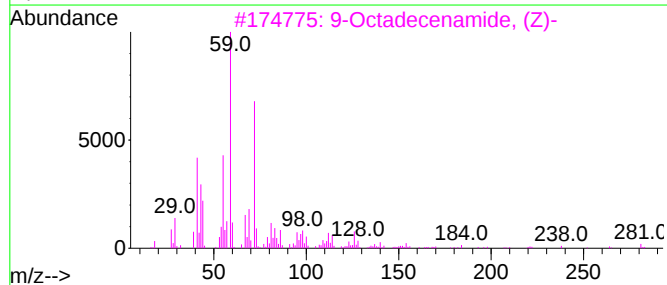
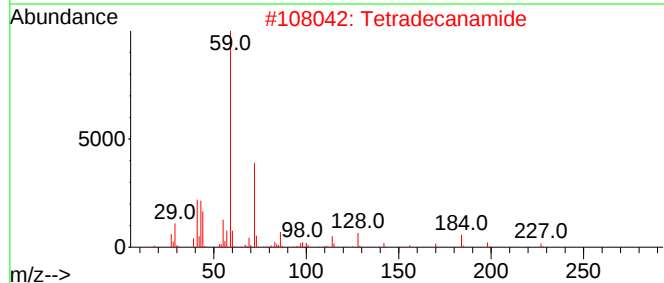
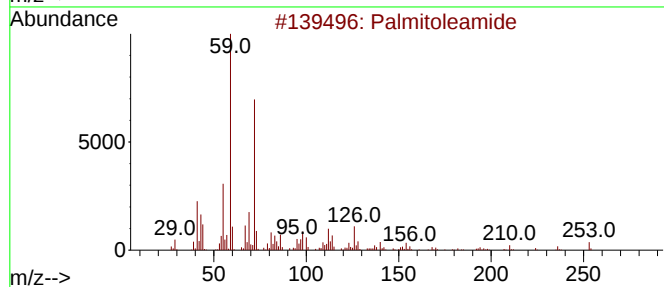
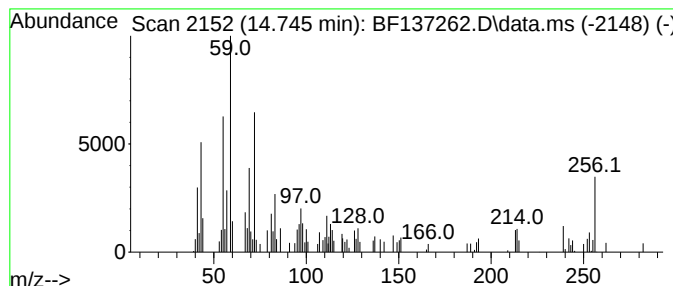
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Palmitoleamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	4.25 ng	62797	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Palmitoleamide	253	C16H31NO	106010-22-4	70
2			Tetradecanamide	227	C14H29NO	000638-58-4	50
3			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	50
4			Hexadecanamide	255	C16H33NO	000629-54-9	50
5			4,5'-Dipyrimidine-2,2'-dithione,...	256	C10H16N4S2	155645-37-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137262.D
Acq On : 02 Feb 2024 18:47
Operator : CG\JU
Sample : P1340-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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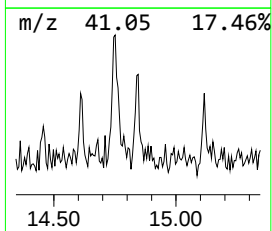
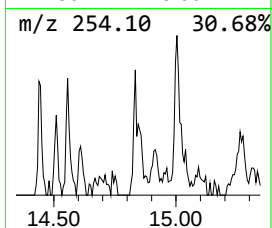
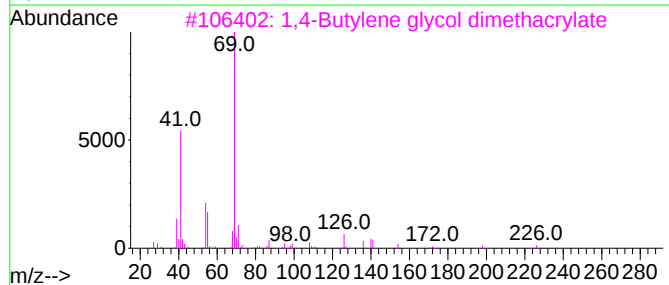
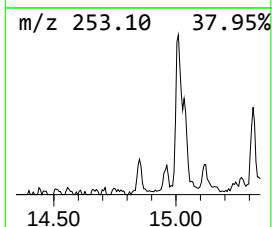
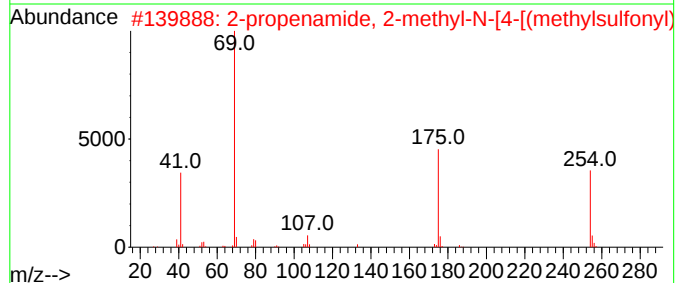
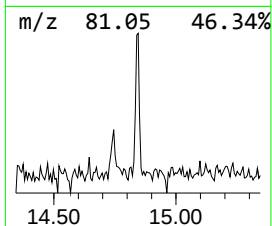
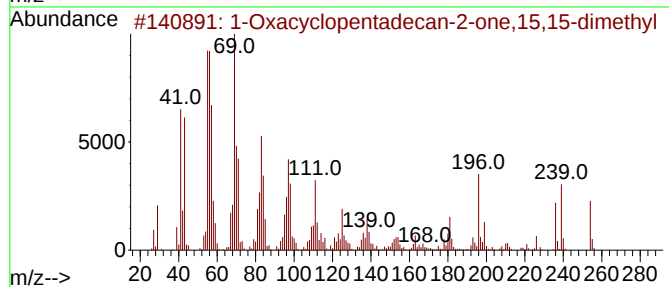
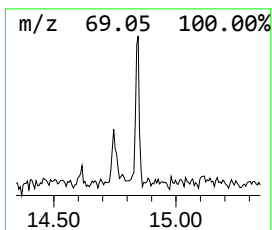
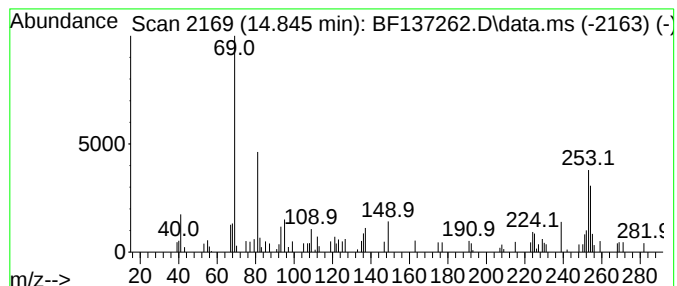
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.845 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	2.36 ng	34853	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Oxacyclopentadecan-2-one,15,15...	254	C16H30O2	1000196-63-1	47		
2	2-propenamide, 2-methyl-N-[4-[(m...	254	C11H14N2O3S	1000401-43-5	47		
3	1,4-Butylene glycol dimethacrylate	226	C12H18O4	002082-81-7	35		
4	.beta.-d-Mannofuranoside, O-geranyl	316	C16H28O6	1000154-77-2	35		
5	Farnesol isomer a	222	C15H26O	1000108-92-4	35		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137262.D
Acq On : 02 Feb 2024 18:47
Operator : CG\JU
Sample : P1340-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

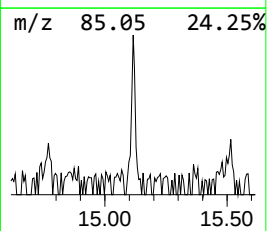
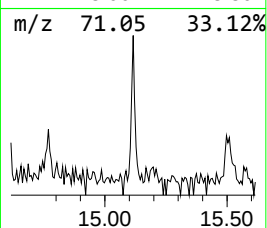
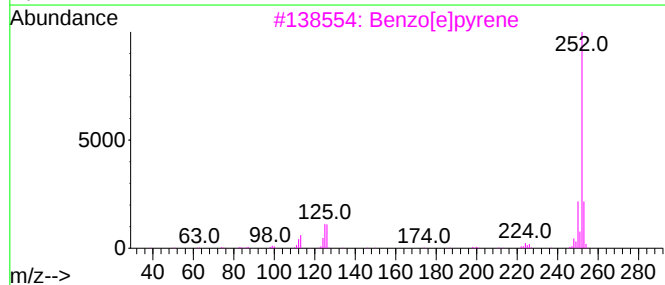
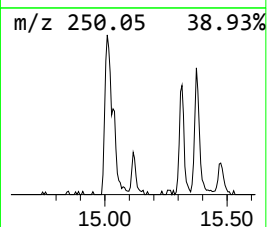
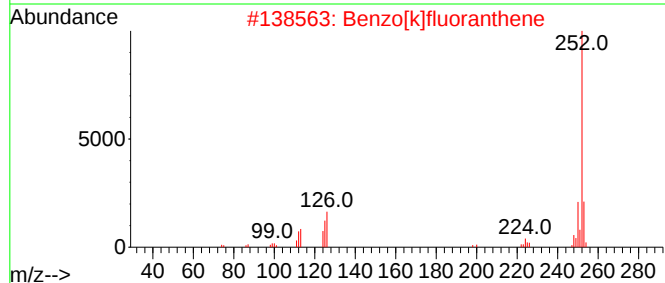
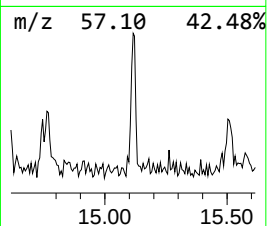
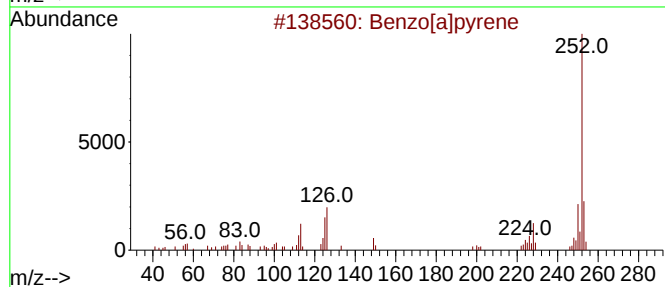
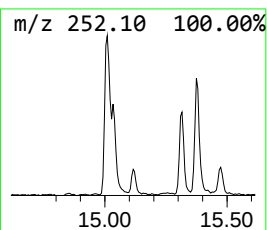
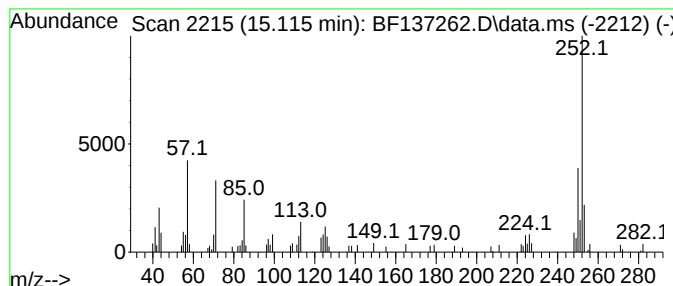
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.116	2.64 ng	39010	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	60
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	60
3			Benzo[e]pyrene	252	C20H12	000192-97-2	53
4			2-Pyridinamine, 3,5-dibromo-	250	C5H4Br2N2	035486-42-1	50
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137262.D
Acq On : 02 Feb 2024 18:47
Operator : CG\JU
Sample : P1340-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

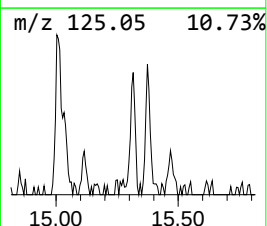
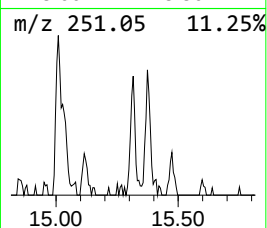
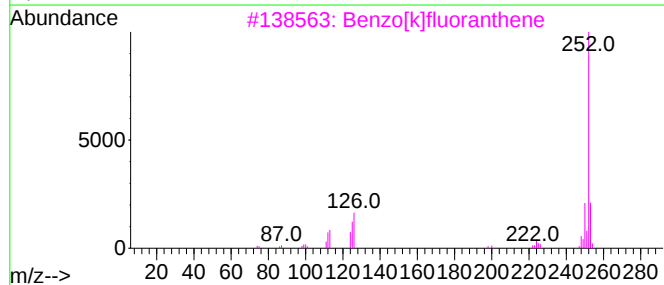
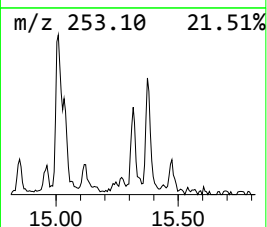
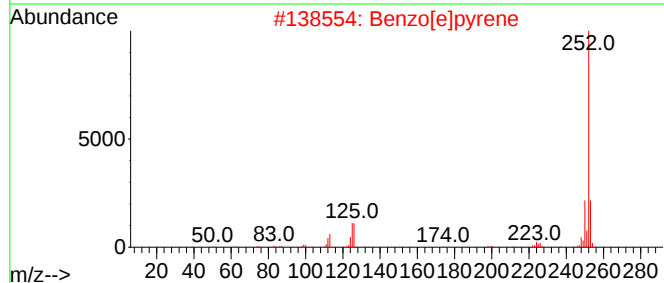
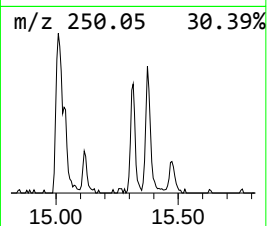
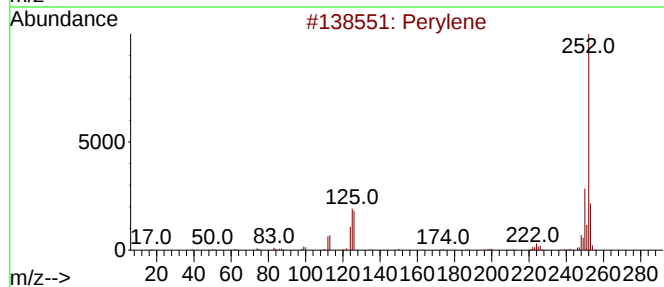
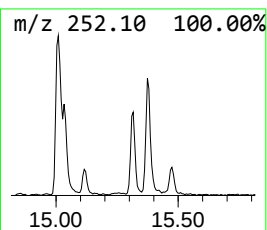
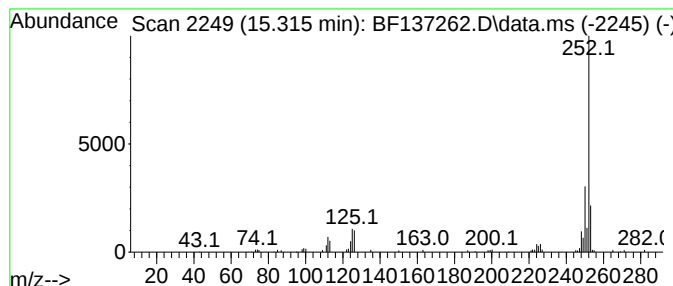
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.315	4.58 ng	67823	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	90
2			Benzo[e]pyrene	252	C20H12	000192-97-2	90
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4			Benzo[a]pyrene	252	C20H12	000050-32-8	81
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137262.D
Acq On : 02 Feb 2024 18:47
Operator : CG\JU
Sample : P1340-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.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
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2-Pentanone, 4-...	5.040	3.0	ng	48841	1	6.792	323116	20.0
n-Hexadecanoic ...	11.851	4.6	ng	100161	4	11.310	434218	20.0
4H-Cyclopenta[d...]	11.927	2.4	ng	52260	4	11.310	434218	20.0
Palmitoleamide	14.745	4.3	ng	62797	6	15.439	295863	20.0
unknown14.845	14.845	2.4	ng	34853	6	15.439	295863	20.0
Benzo[e]pyrene	15.116	2.6	ng	39010	6	15.439	295863	20.0
Perylene	15.315	4.6	ng	67823	6	15.439	295863	20.0