

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
 Data File : BF125976.D
 Acq On : 27 Oct 2021 21:58
 Operator : JU/CG
 Sample : M4367-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-102621

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-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125976.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	14	rVB	2931479	3908661	44.96%	6.923%
2	5.469	570	575	579	rBV	4394131	4678345	53.82%	8.286%
3	6.481	741	747	750	rBV	4636925	4652083	53.51%	8.239%
4	6.687	779	782	787	rBV2	90738	128131	1.47%	0.227%
5	6.857	807	811	814	rBV	1553167	1183583	13.62%	2.096%
6	7.416	898	906	909	rBV	3253826	3057939	35.18%	5.416%
7	7.457	909	913	916	rVB	119901	106054	1.22%	0.188%
8	8.045	1009	1013	1020	rBV	1472216	1341223	15.43%	2.375%
9	8.139	1024	1029	1032	rVV	1884470	1660985	19.11%	2.942%
10	8.733	1127	1130	1134	rBV	187604	147188	1.69%	0.261%
11	9.216	1207	1212	1215	rBV	5407441	4739856	54.52%	8.395%
12	9.298	1223	1226	1230	rBV	211052	179918	2.07%	0.319%
13	9.622	1276	1281	1283	rBV2	71740	91607	1.05%	0.162%
14	9.828	1314	1316	1320	rVB	197229	150774	1.73%	0.267%
15	9.892	1323	1327	1330	rVB	2060564	1660007	19.10%	2.940%
16	10.327	1398	1401	1404	rVB	204055	146425	1.68%	0.259%
17	10.675	1456	1460	1464	rVB	2860818	2649313	30.48%	4.692%
18	10.798	1479	1481	1490	rVB	176234	234207	2.69%	0.415%
19	11.251	1555	1558	1560	rBV	154669	122896	1.41%	0.218%
20	11.374	1575	1579	1582	rBV	1805677	1521222	17.50%	2.694%
21	11.674	1627	1630	1633	rBV	138289	112501	1.29%	0.199%
22	11.774	1644	1647	1650	rBV	3063088	2364233	27.20%	4.187%
23	11.904	1666	1669	1673	rVB	261987	201939	2.32%	0.358%
24	12.080	1696	1699	1706	rVB2	100038	125049	1.44%	0.221%
25	12.469	1760	1765	1767	rBV	7545927	8693190	100.00%	15.397%
26	12.486	1767	1768	1774	rVB2	5805456	4165608	47.92%	7.378%
27	12.569	1779	1782	1788	rVB2	1195679	1104902	12.71%	1.957%
28	12.816	1818	1824	1826	rBV	311691	296346	3.41%	0.525%
29	12.963	1845	1849	1852	rBV	4074706	3641790	41.89%	6.450%
30	13.145	1873	1880	1883	rBV3	60393	112470	1.29%	0.199%
31	13.204	1887	1890	1894	rVB3	69668	115819	1.33%	0.205%
32	13.868	1999	2003	2011	rVB2	277655	345678	3.98%	0.612%
33	14.010	2022	2027	2030	rBV	1336304	1364207	15.69%	2.416%
34	14.033	2030	2031	2034	rVB	145851	107968	1.24%	0.191%
35	15.051	2200	2204	2207	rBV2	108413	182829	2.10%	0.324%
36	15.351	2252	2255	2259	rVB	89457	101371	1.17%	0.180%

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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-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.410	2262	2265	2270	rVB	110909	118309	1.36%	0.210%
38	15.474	2272	2276	2280	rBV	814650	946657	10.89%	1.677%

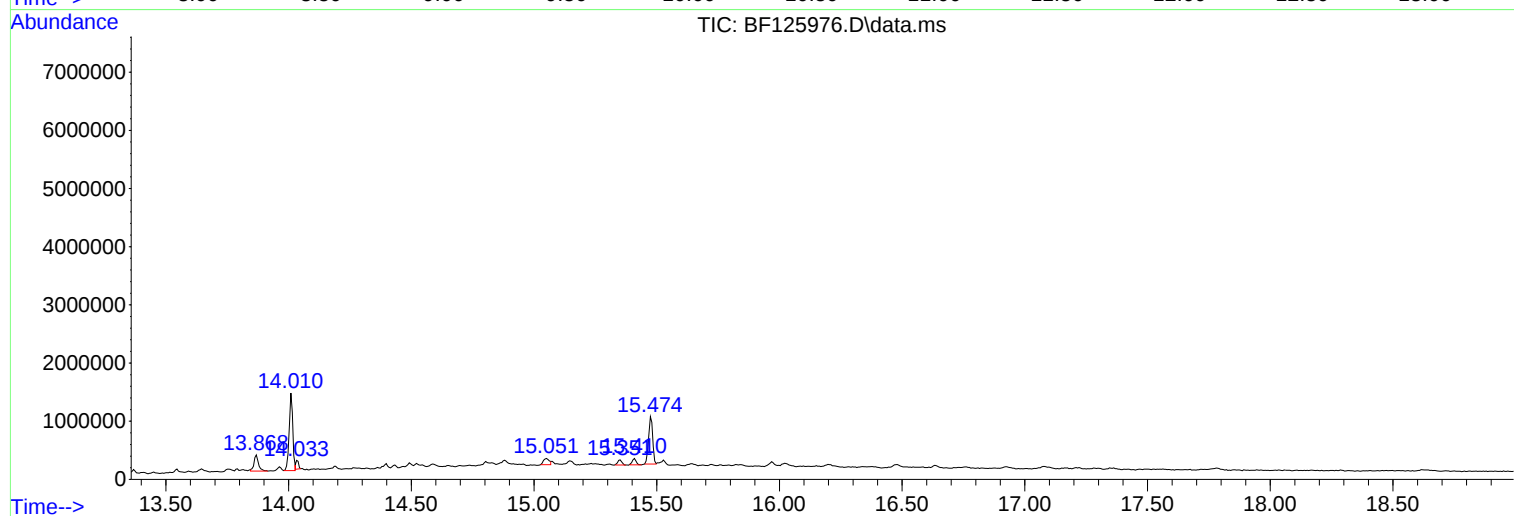
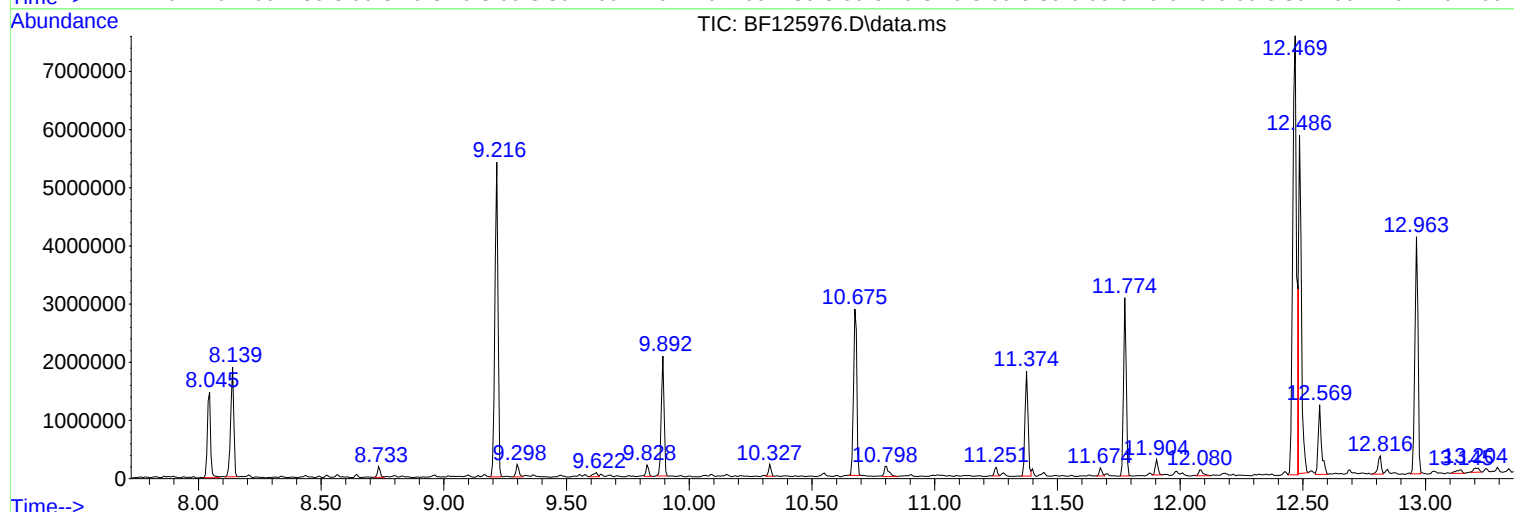
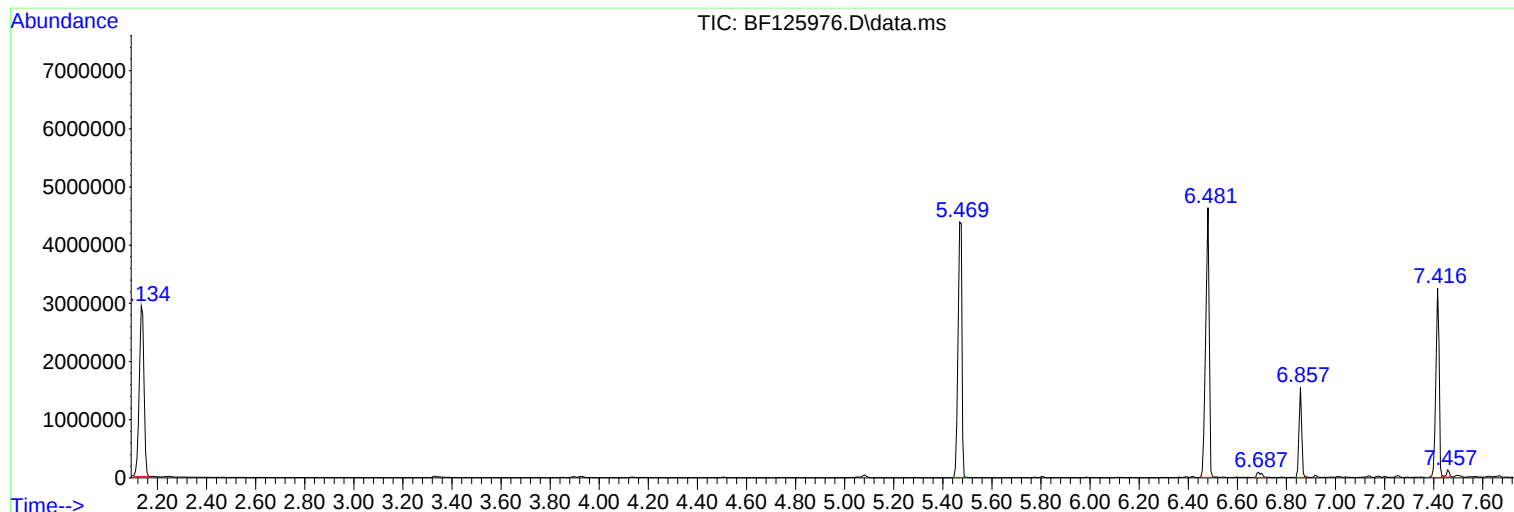
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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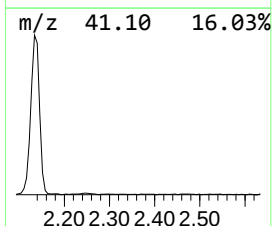
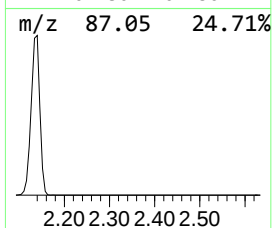
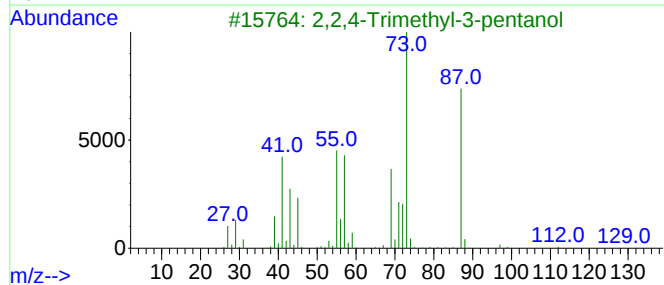
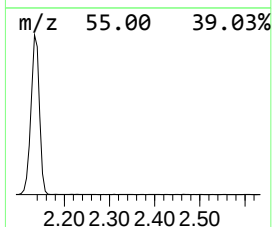
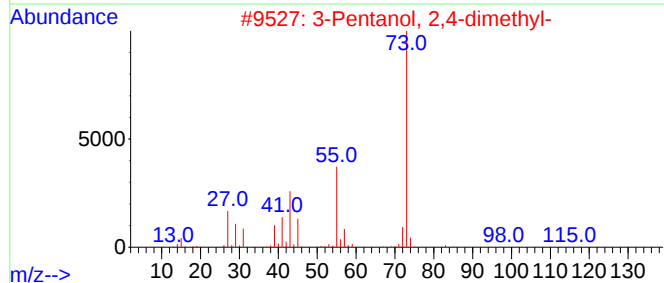
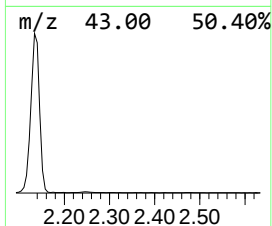
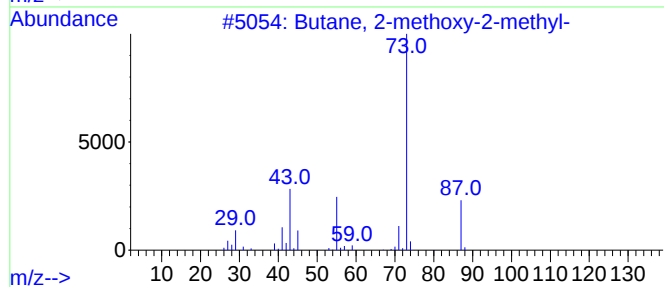
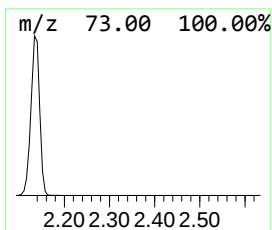
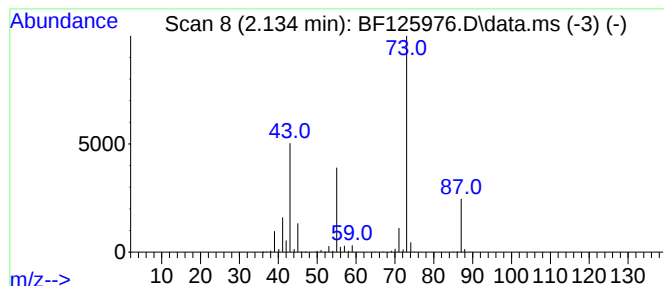
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	66.05 ng	3908660	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23



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Instrument :
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ClientSampleId :
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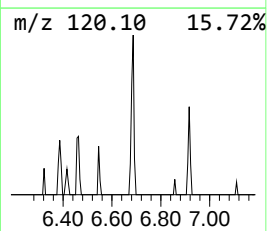
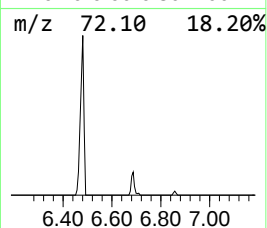
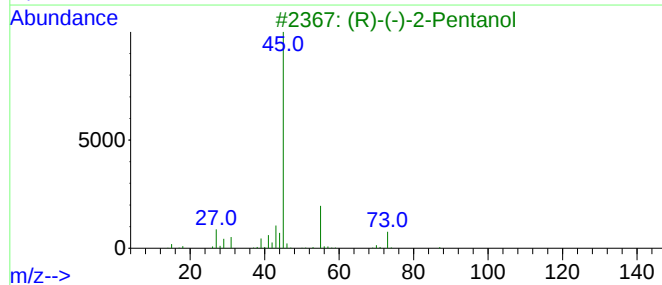
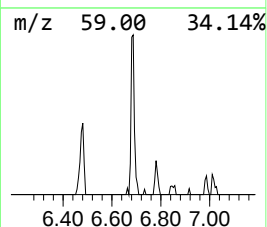
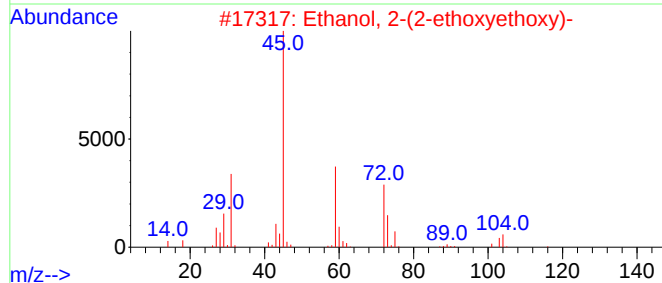
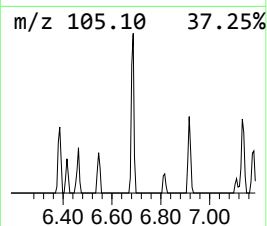
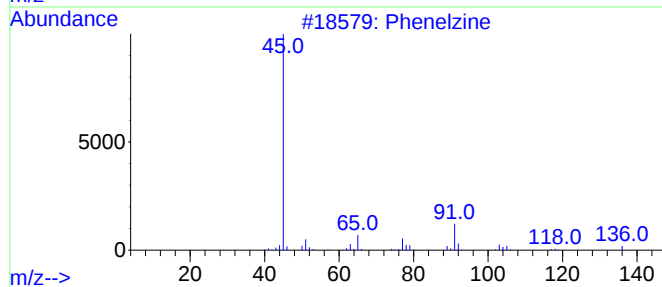
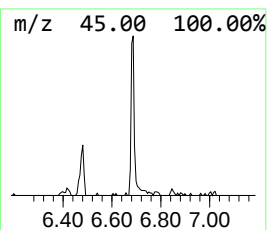
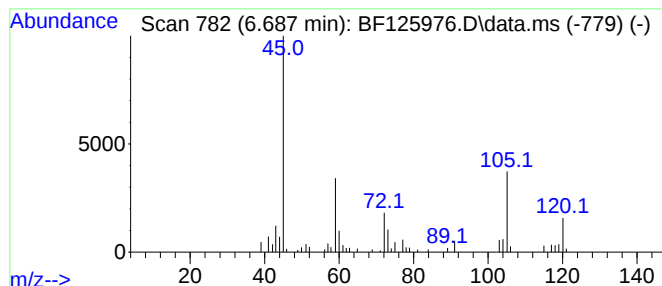
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Peak Number 2 unknown6.687 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.687	2.17 ng	128131	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenelzine	136	C8H12N2	000051-71-8	38
2			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	38
3			(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	32
4			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	28
5			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	28



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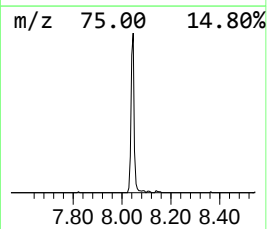
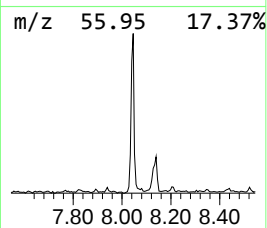
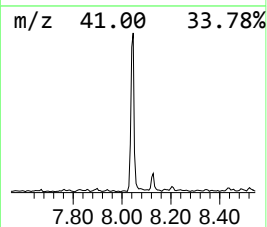
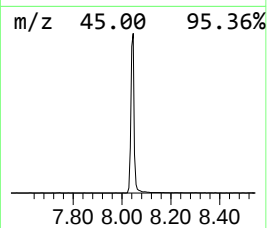
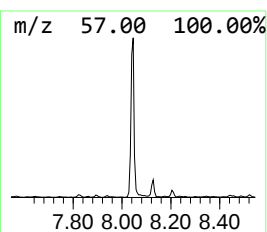
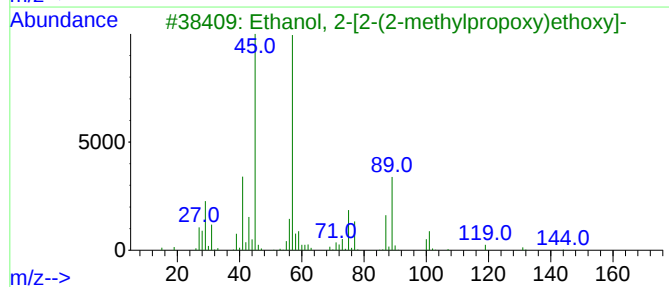
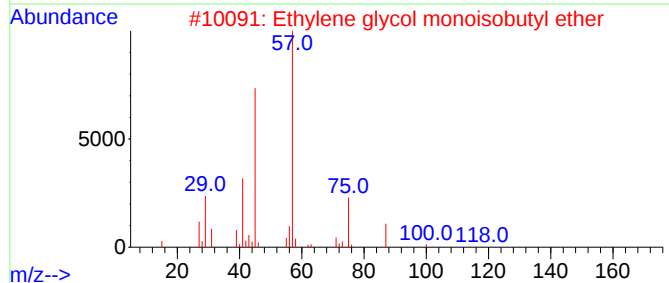
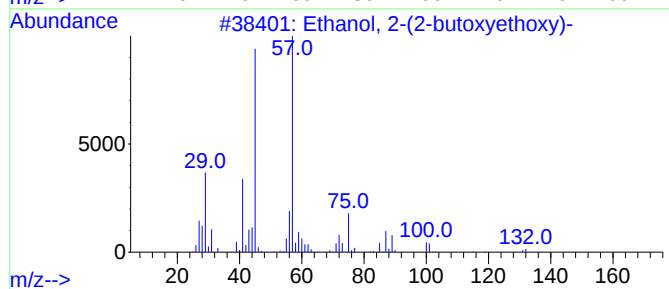
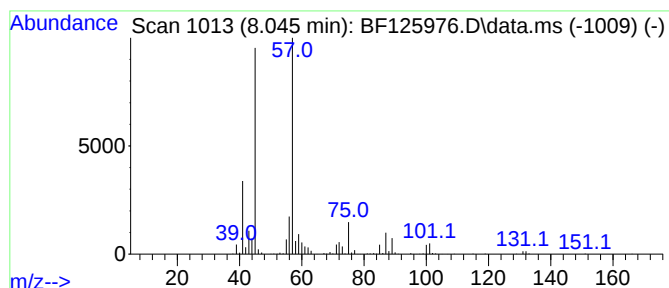
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.045	16.15 ng	1341220	Naphthalene-d8	8.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Pentaethylene glycol	238	C10H22O6	004792-15-8	53



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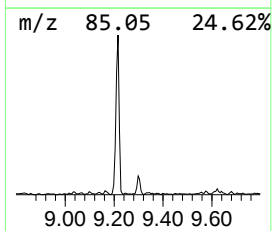
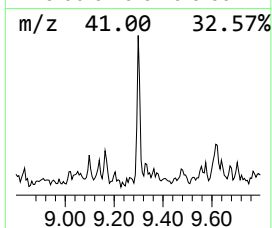
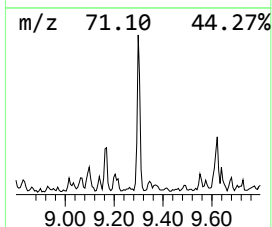
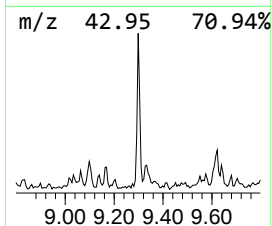
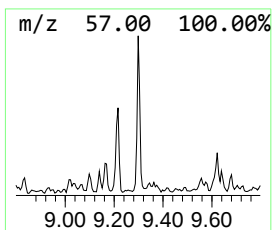
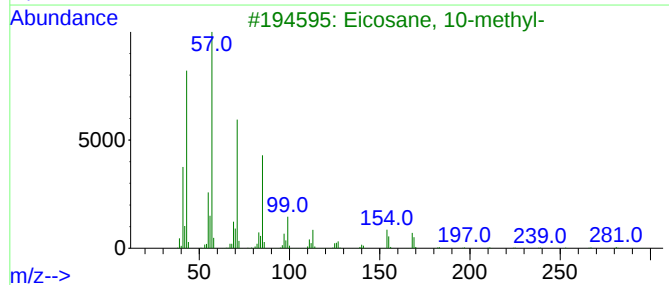
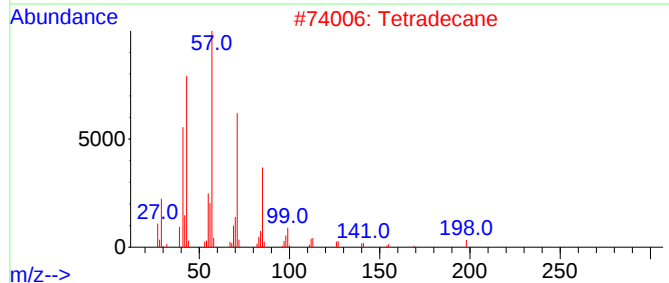
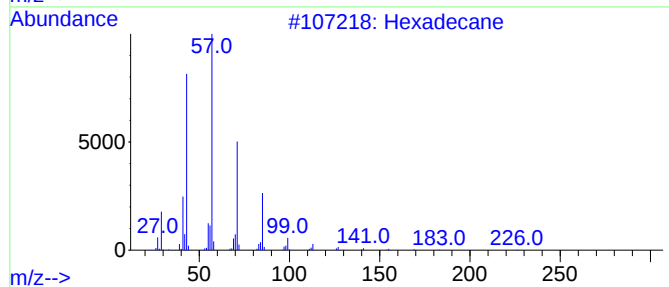
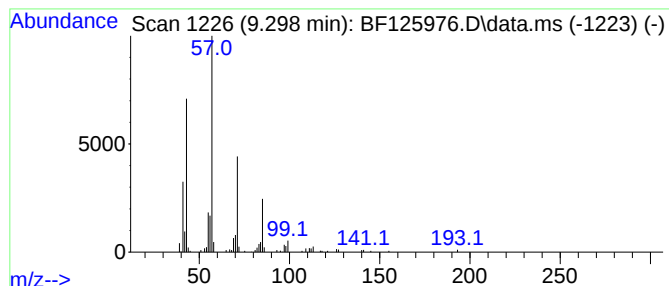
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Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.298	2.17 ng	179918	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Tetradecane	198	C14H30	000629-59-4	80
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
4			Heptadecane	240	C17H36	000629-78-7	78
5			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	72



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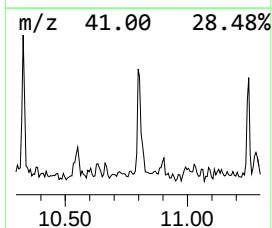
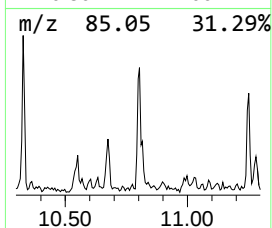
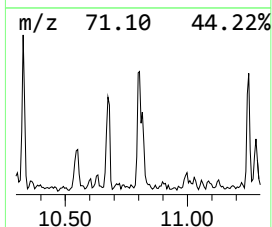
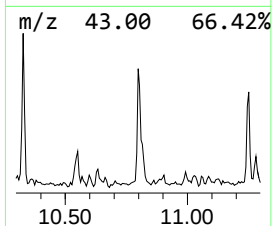
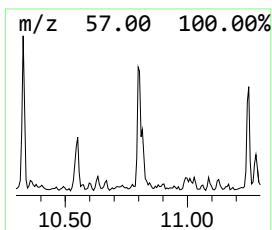
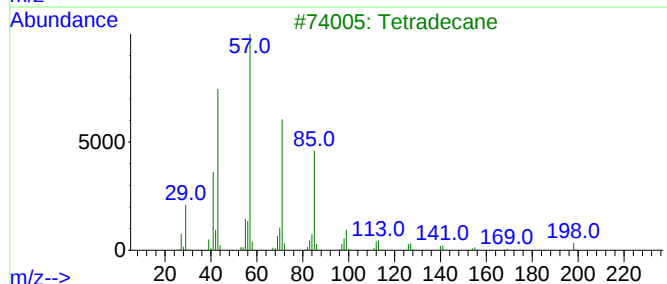
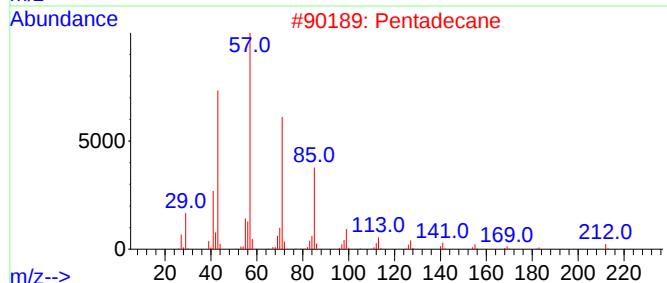
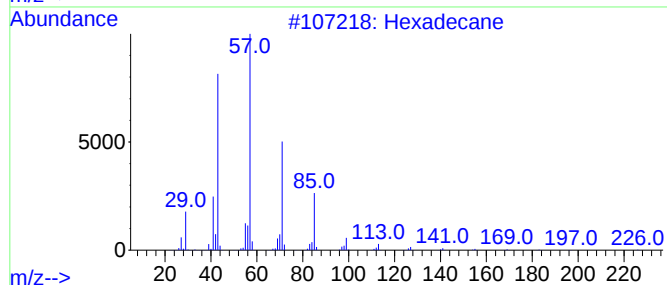
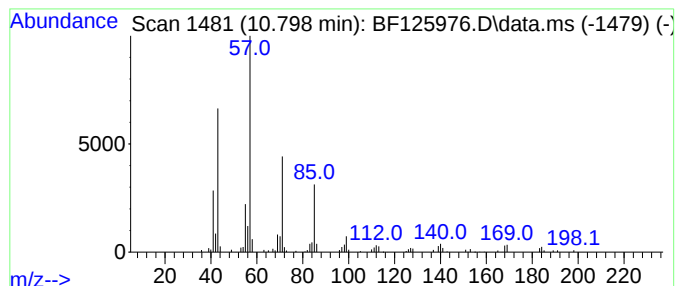
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	3.08 ng	234207	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	87
2			Pentadecane	212	C15H32	000629-62-9	86
3			Tetradecane	198	C14H30	000629-59-4	86
4			Tridecane	184	C13H28	000629-50-5	81
5			Tridecane, 6-methyl-	198	C14H30	013287-21-3	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125976.D
Acq On : 27 Oct 2021 21:58
Operator : JU/CG
Sample : M4367-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-102621

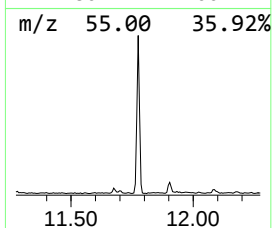
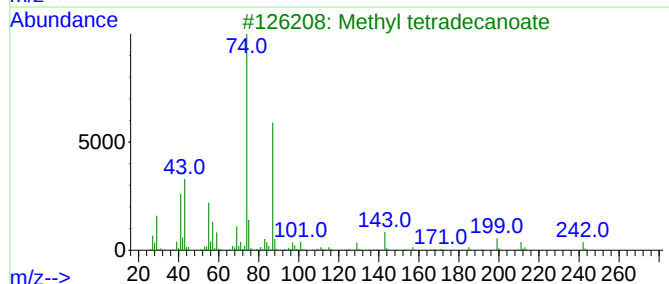
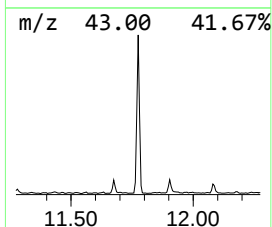
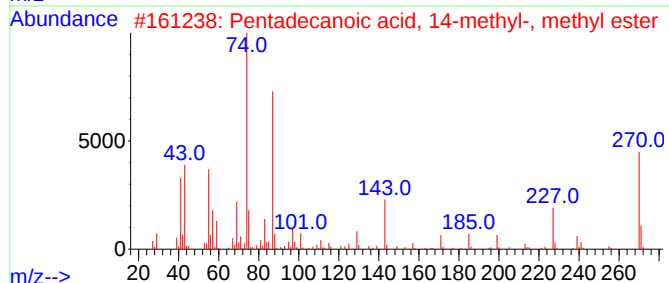
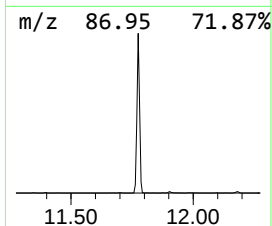
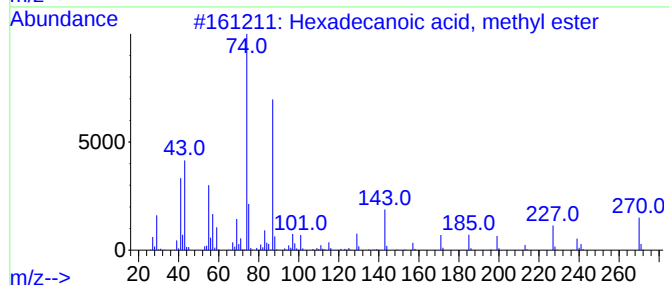
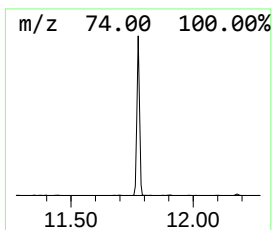
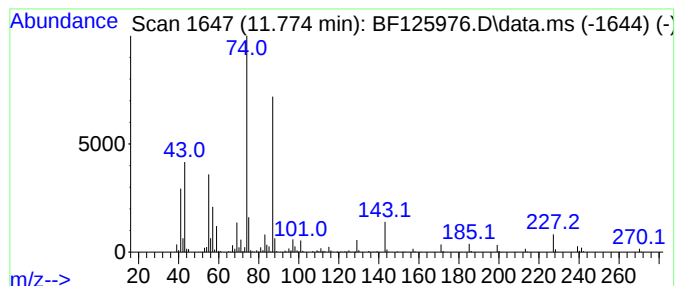
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.774	31.08 ng	2364230	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125976.D
Acq On : 27 Oct 2021 21:58
Operator : JU/CG
Sample : M4367-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-102621

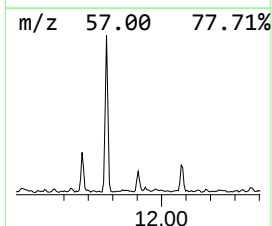
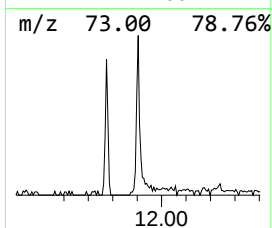
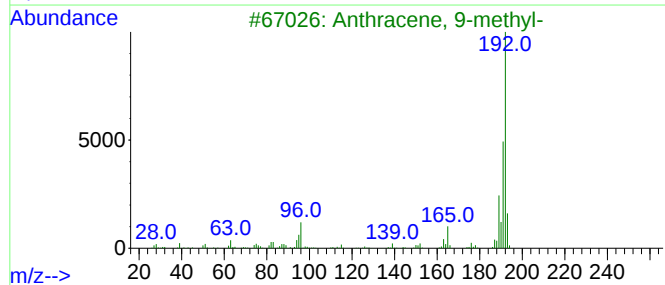
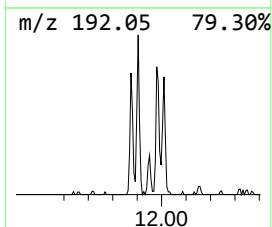
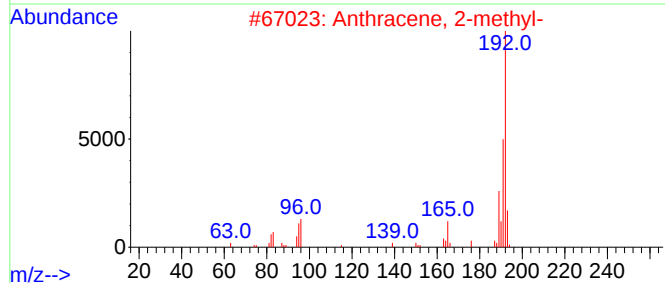
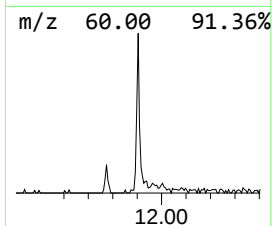
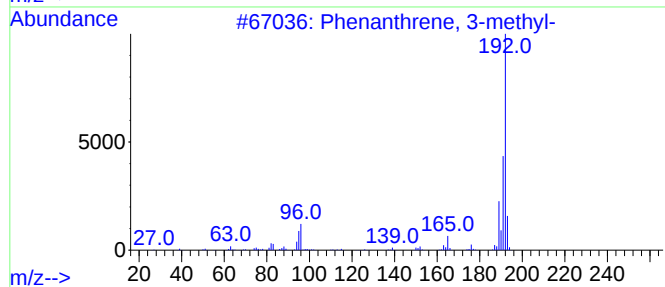
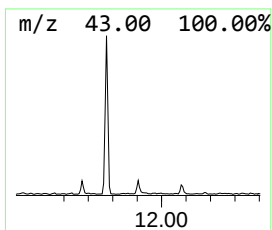
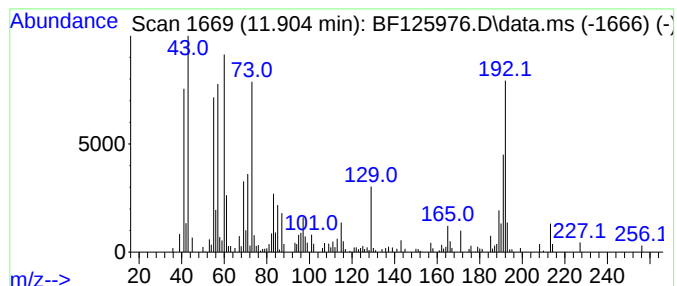
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenanthrene, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	2.65 ng	201939	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	70
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	70
3			Anthracene, 9-methyl-	192	C15H12	000779-02-2	55
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	52
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125976.D
Acq On : 27 Oct 2021 21:58
Operator : JU/CG
Sample : M4367-01
Misc :
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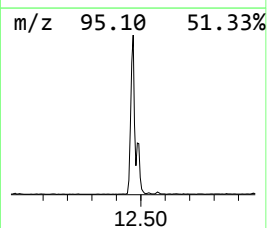
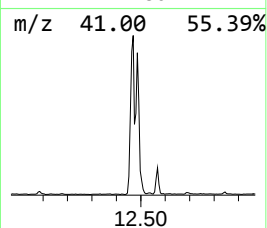
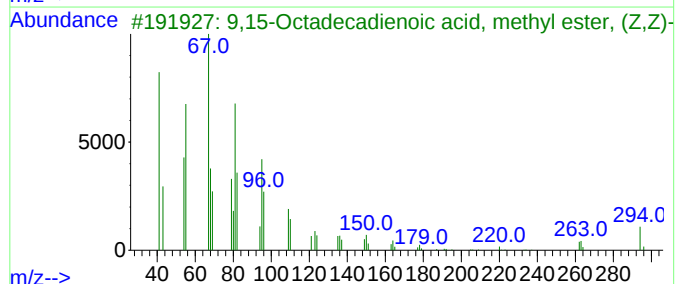
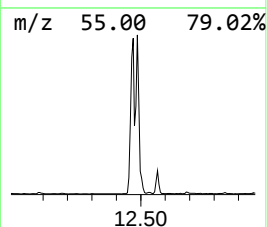
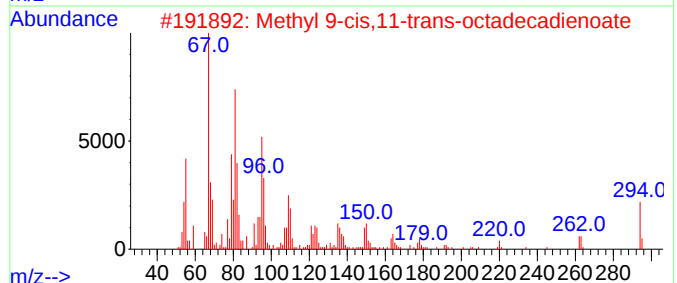
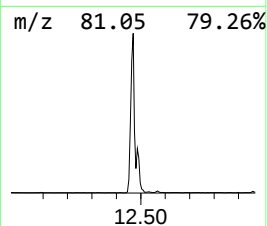
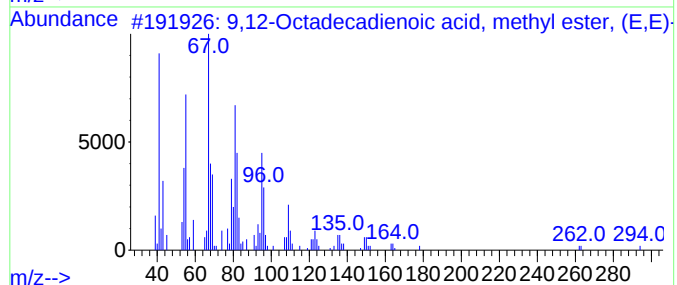
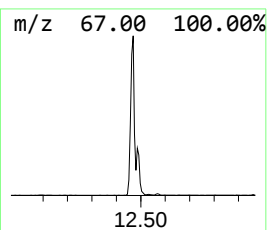
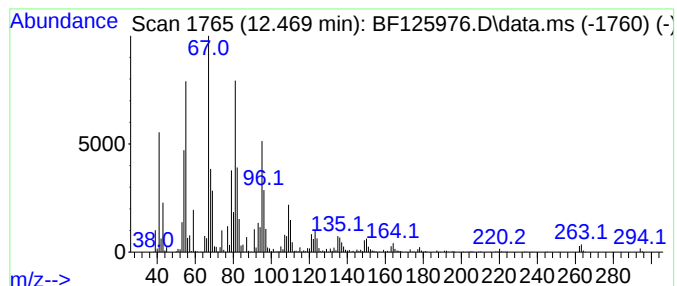
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.469	114.29 ng	8693190	Phenanthrene-d10	11.374	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125976.D
Acq On : 27 Oct 2021 21:58
Operator : JU/CG
Sample : M4367-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-05-102621

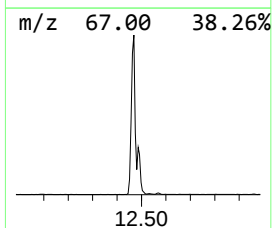
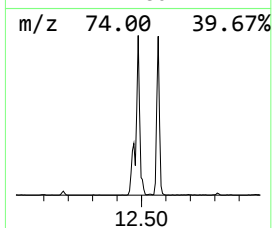
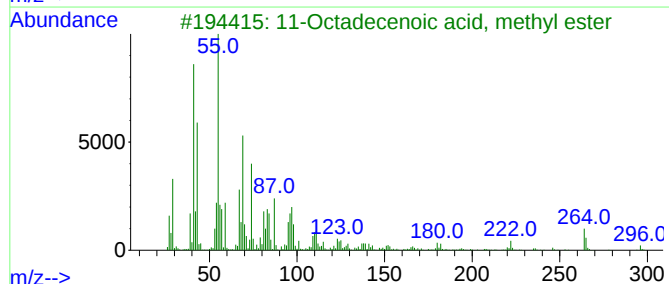
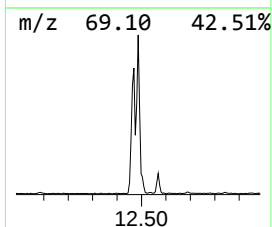
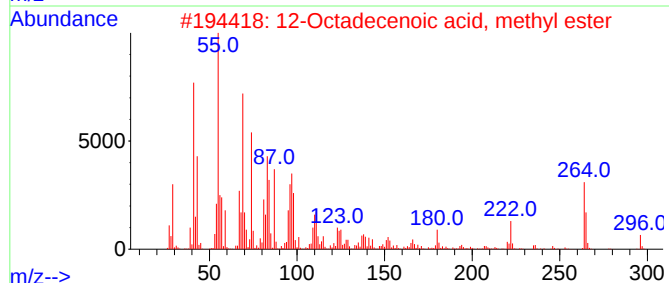
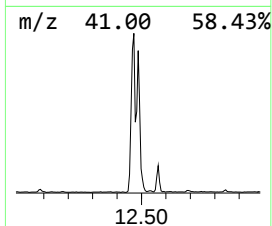
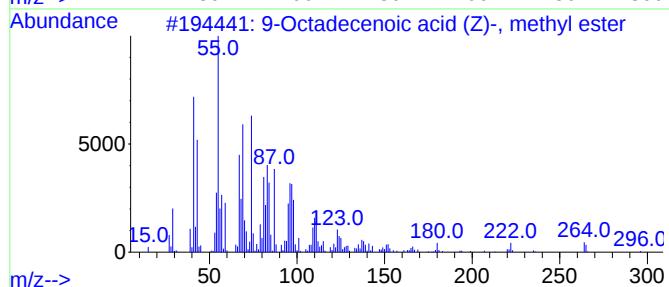
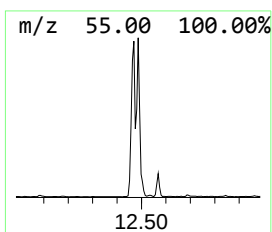
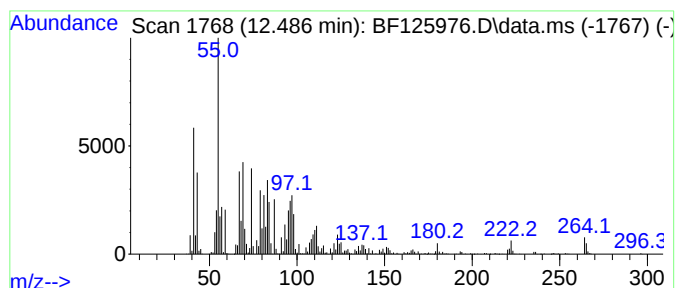
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.486	54.77 ng	4165610	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99		
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	98		
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	91		
4	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	91		
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125976.D
Acq On : 27 Oct 2021 21:58
Operator : JU/CG
Sample : M4367-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

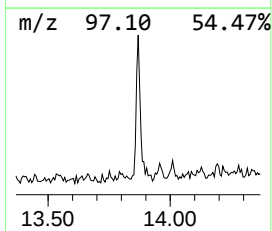
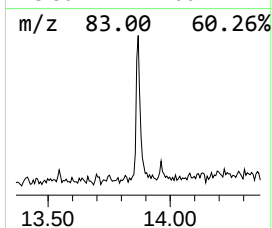
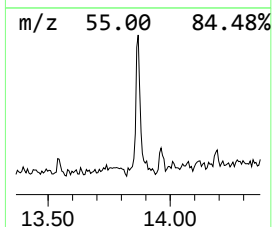
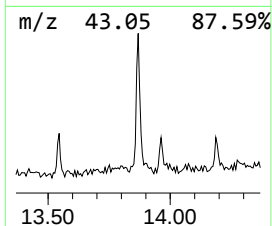
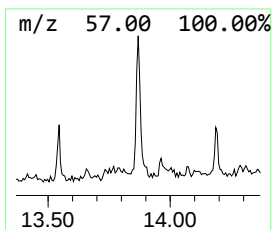
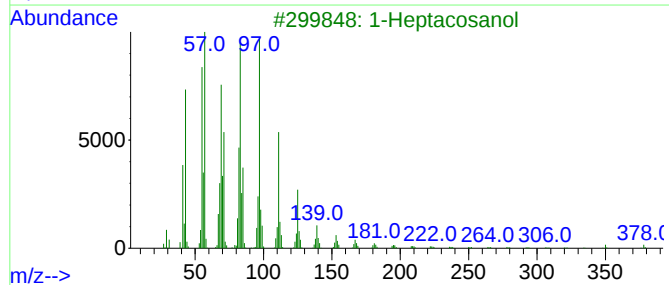
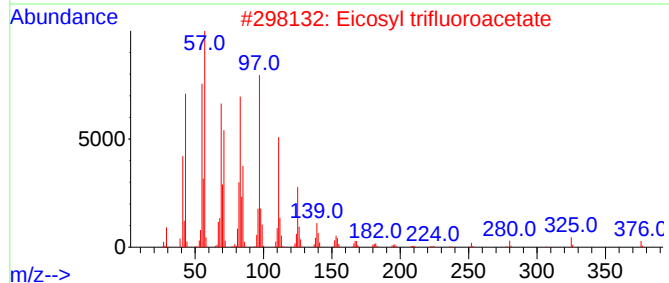
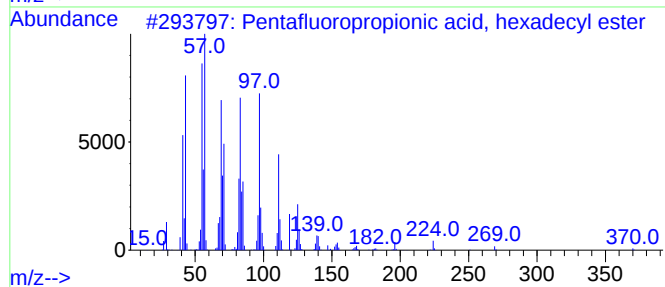
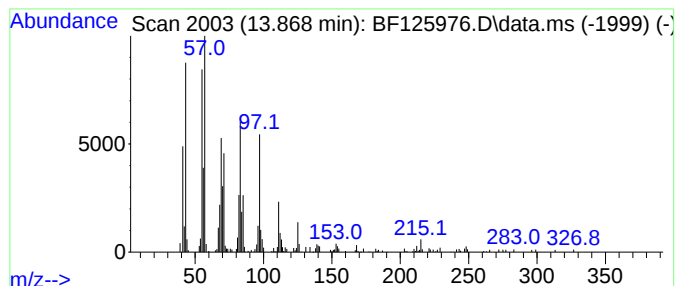
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.868	5.07 ng	345678	Chrysene-d12			14.010
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
2		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		Pentafluoropropionic acid, heptacosyl ester	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125976.D
Acq On : 27 Oct 2021 21:58
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-05-102621

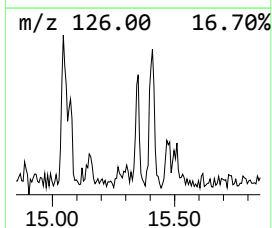
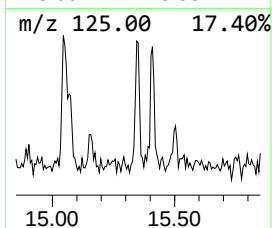
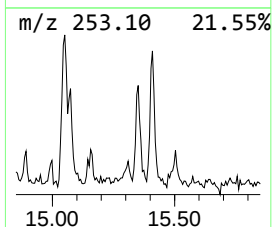
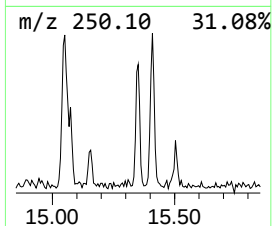
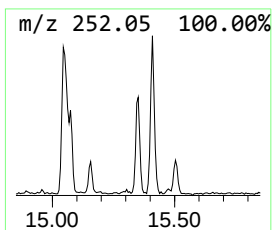
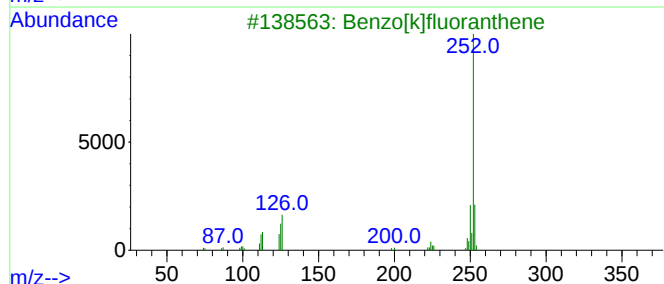
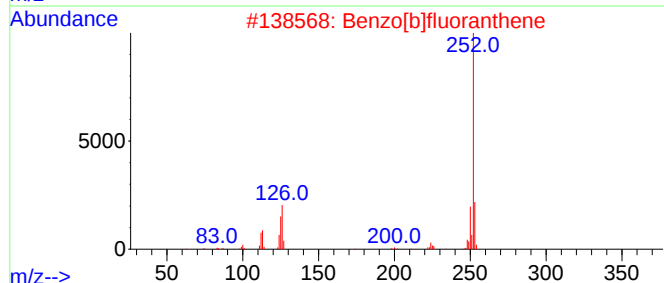
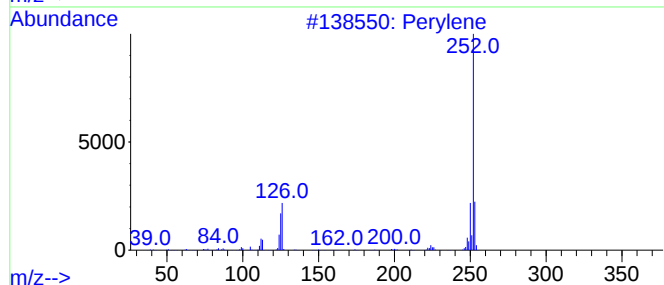
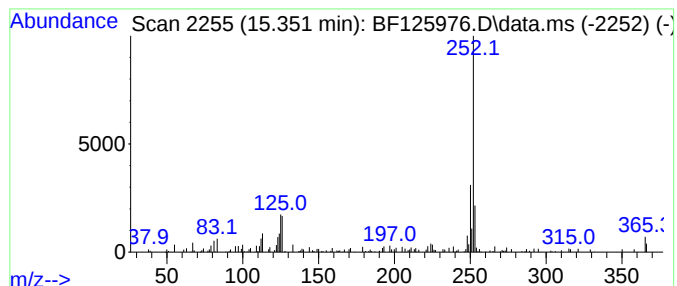
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Perylene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	2.14 ng	101371	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	95
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[e]pyrene	252	C20H12	000192-97-2	90
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102721\
Data File : BF125976.D
Acq On : 27 Oct 2021 21:58
Operator : JU/CG
Sample : M4367-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-102621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.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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unknown6.687	6.687	2.2	ng	128131	1	6.857	1183580	20.0
Ethanol, 2-(2-b...	8.045	16.1	ng	1341220	2	8.139	1660990	20.0
Hexadecane	9.298	2.2	ng	179918	3	9.892	1660010	20.0
Pentadecane	10.798	3.1	ng	234207	4	11.374	1521220	20.0
Hexadecanoic ac...	11.774	31.1	ng	2364230	4	11.374	1521220	20.0
Phenanthrene, 3...	11.904	2.6	ng	201939	4	11.374	1521220	20.0
9,12-Octadecadi...	12.469	114.3	ng	8693190	4	11.374	1521220	20.0
9-Octadecenoic ...	12.486	54.8	ng	4165610	4	11.374	1521220	20.0
Pentafluoroprop...	13.868	5.1	ng	345678	5	14.010	1364210	20.0
Perylene	15.351	2.1	ng	101371	6	15.474	946657	20.0