

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
 Data File : BF125111.D
 Acq On : 19 Aug 2021 13:22
 Operator : JU/CG
 Sample : M3442-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 210812088-01

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	16	22	28	rVB	2385413	3063070	62.88%	11.695%
2	5.128	513	517	521	rBV	387920	343300	7.05%	1.311%
3	6.916	818	821	825	rVB	1268738	1004591	20.62%	3.836%
4	7.481	911	917	920	rBV	3175993	3037717	62.35%	11.599%
5	8.098	1019	1022	1035	rBV	466059	518386	10.64%	1.979%
6	8.198	1035	1039	1043	rVB	1549188	1312989	26.95%	5.013%
7	9.280	1217	1223	1226	rBV	4842017	4871651	100.00%	18.601%
8	9.957	1334	1338	1341	rBV	1778836	1458810	29.94%	5.570%
9	10.139	1361	1369	1377	rBV2	40719	78464	1.61%	0.300%
10	10.563	1433	1441	1446	rBV3	25265	63530	1.30%	0.243%
11	11.098	1525	1532	1540	rBV3	23391	64257	1.32%	0.245%
12	11.445	1587	1591	1594	rBV	1681161	1521273	31.23%	5.808%
13	11.963	1674	1679	1690	rBV2	570577	737559	15.14%	2.816%
14	12.110	1701	1704	1708	rBV	65185	63766	1.31%	0.243%
15	12.174	1710	1715	1718	rVV3	122100	121648	2.50%	0.464%
16	12.745	1808	1812	1823	rBV	262423	326988	6.71%	1.249%
17	12.886	1826	1836	1846	rVB3	141372	351110	7.21%	1.341%
18	13.027	1856	1860	1864	rVB	3602517	3537155	72.61%	13.506%
19	13.298	1900	1906	1911	rVB2	56263	109021	2.24%	0.416%
20	13.945	2010	2016	2028	rBV	169532	335846	6.89%	1.282%
21	14.080	2035	2039	2043	rVB	1325103	1170461	24.03%	4.469%
22	14.486	2104	2108	2114	rVB	124188	154530	3.17%	0.590%
23	14.862	2169	2172	2177	rVB	54549	58169	1.19%	0.222%
24	14.998	2190	2195	2202	rBV2	87521	147344	3.02%	0.563%
25	15.062	2202	2206	2213	rVV9	31171	55409	1.14%	0.212%
26	15.215	2228	2232	2237	rVB	53037	59422	1.22%	0.227%
27	15.392	2255	2262	2272	rBV	39461	120123	2.47%	0.459%
28	15.580	2288	2294	2305	rBV	794368	1168321	23.98%	4.461%
29	16.062	2372	2376	2382	rVB2	33484	53003	1.09%	0.202%
30	16.239	2401	2406	2414	rVB3	42427	93807	1.93%	0.358%
31	17.027	2535	2540	2548	rVB5	24925	57924	1.19%	0.221%
32	17.439	2604	2610	2620	rVB5	24459	68269	1.40%	0.261%
33	17.933	2691	2694	2703	rVB5	25233	62554	1.28%	0.239%

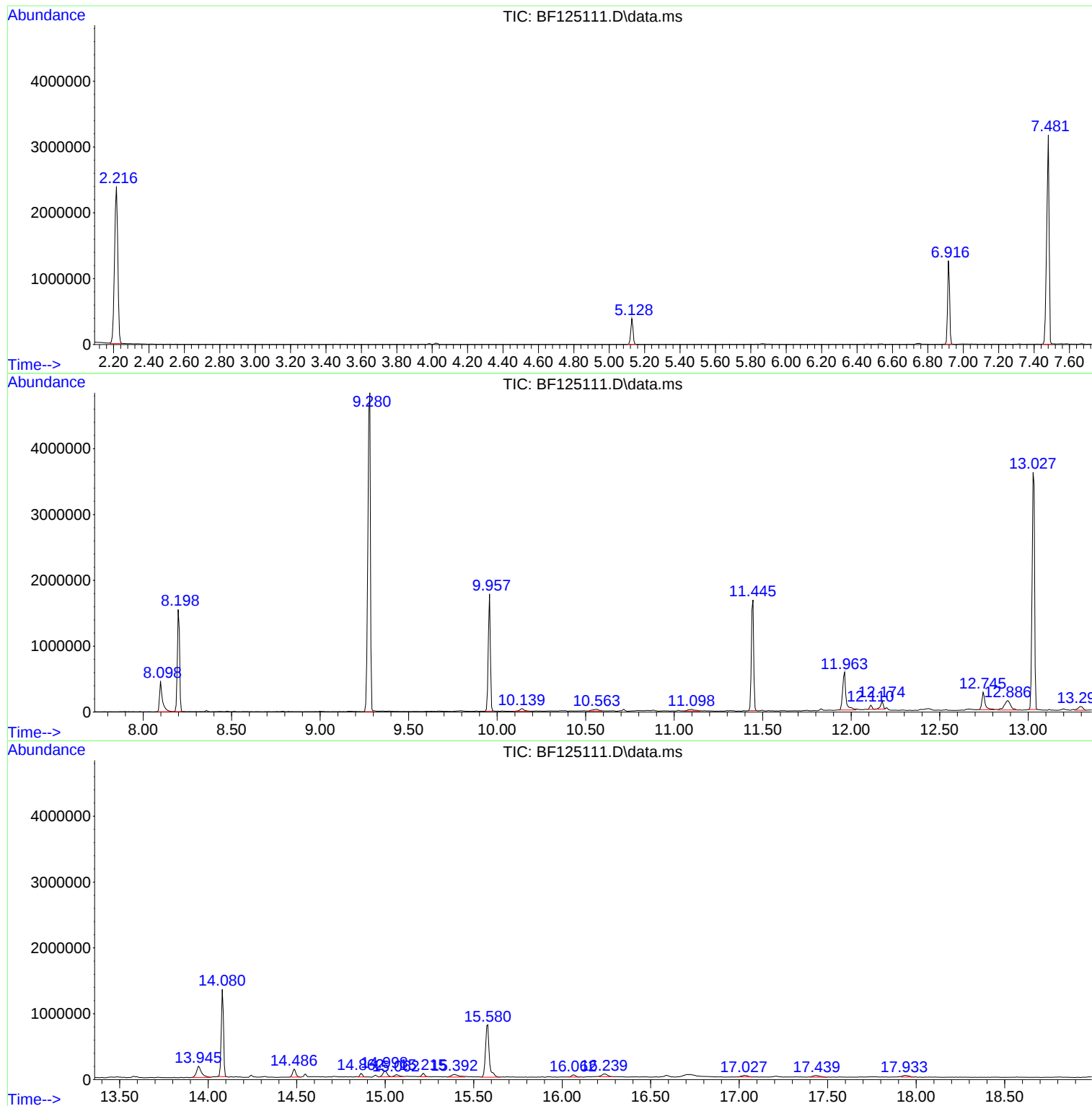
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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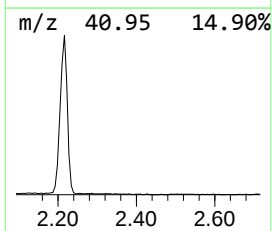
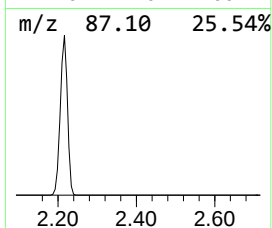
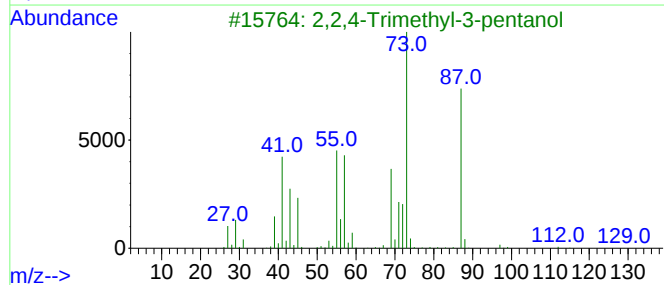
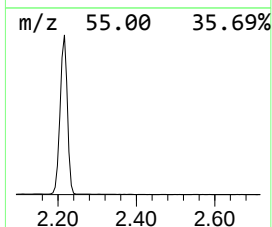
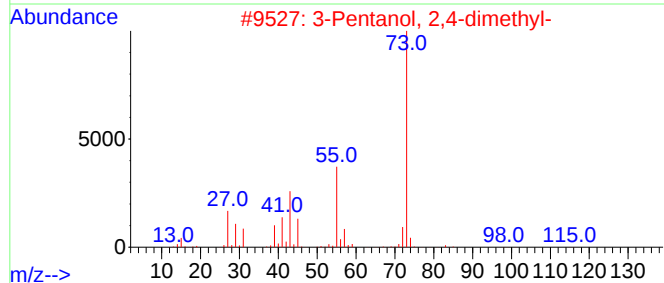
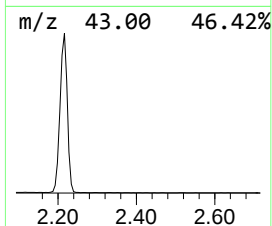
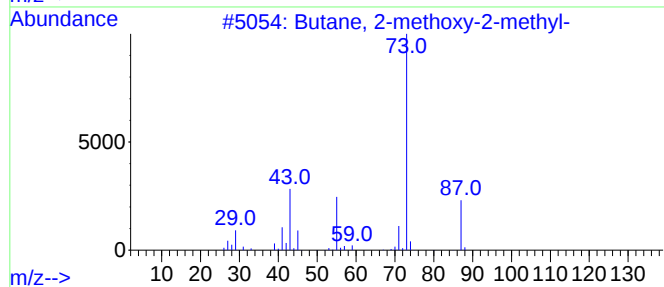
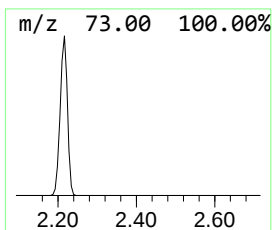
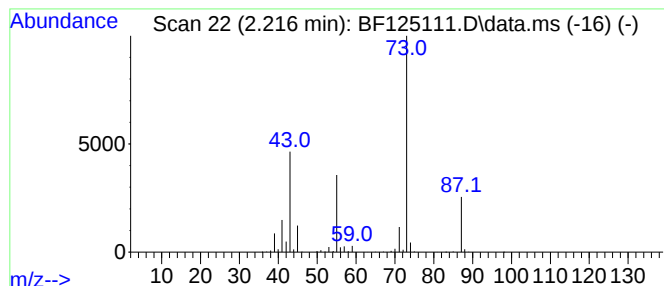
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	60.98 ng	3063070	1,4-Dichlorobenzene-d4	6.916

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	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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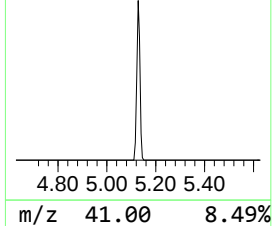
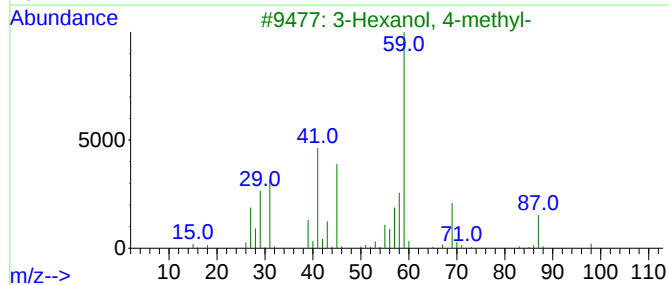
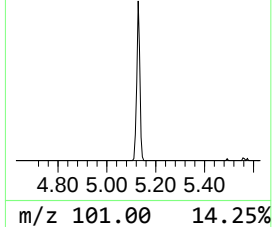
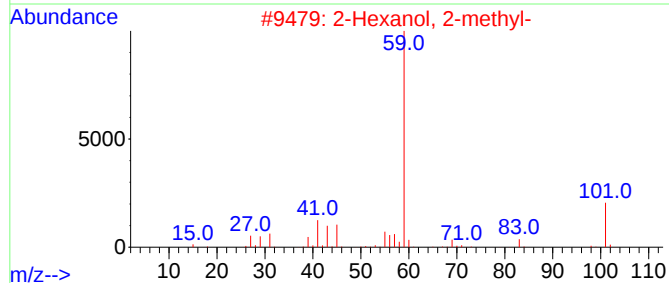
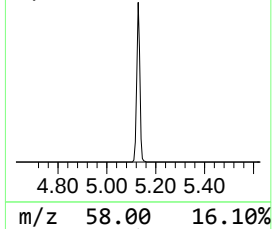
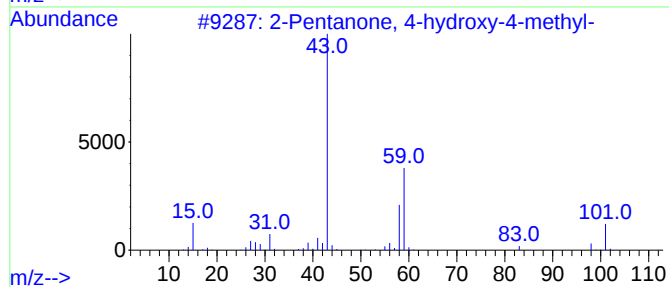
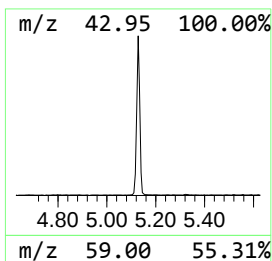
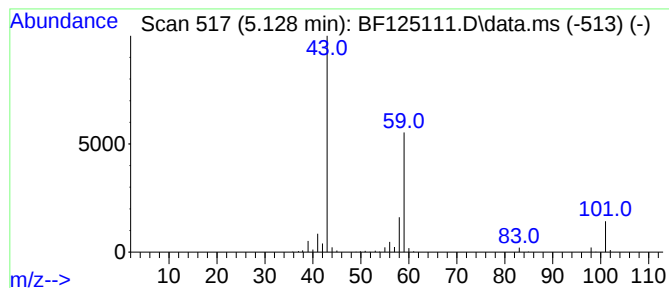
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	6.83 ng	343300	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			3-Octanol	130	C8H18O	000589-98-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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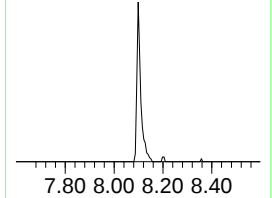
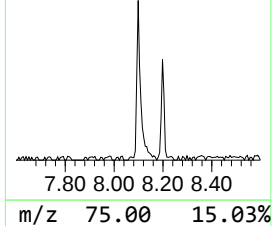
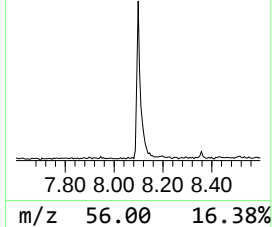
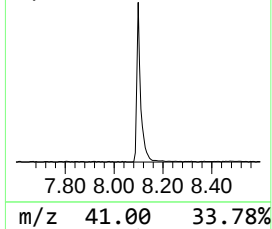
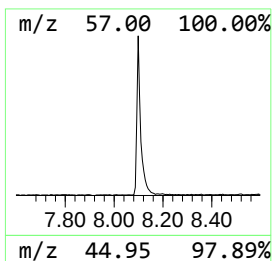
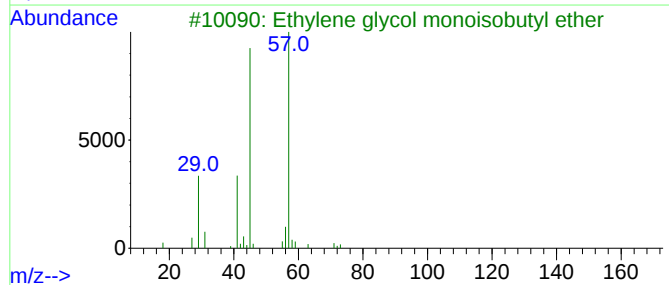
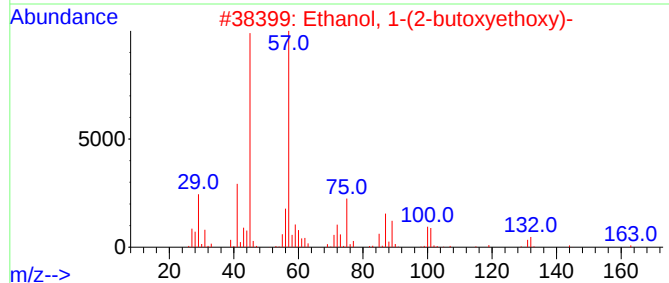
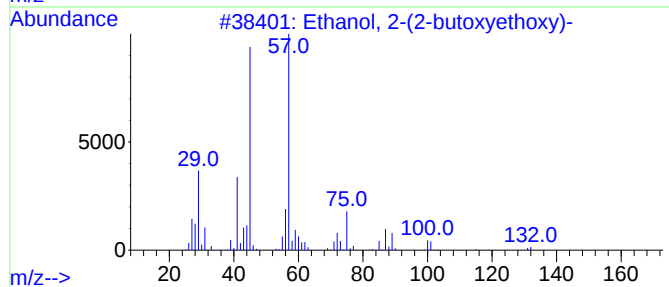
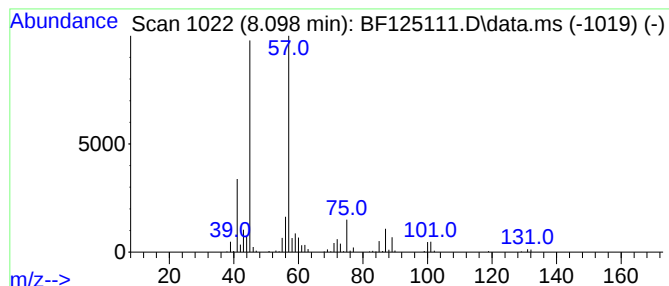
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	7.90 ng	518386	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Butyl lactate	146	C7H14O3	000138-22-7	47



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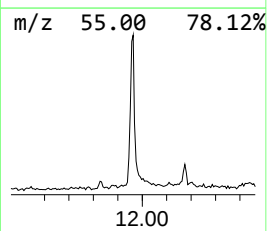
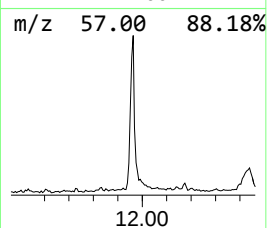
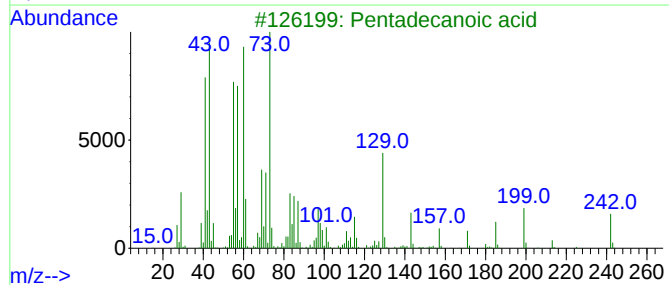
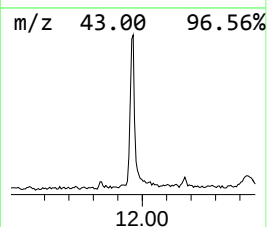
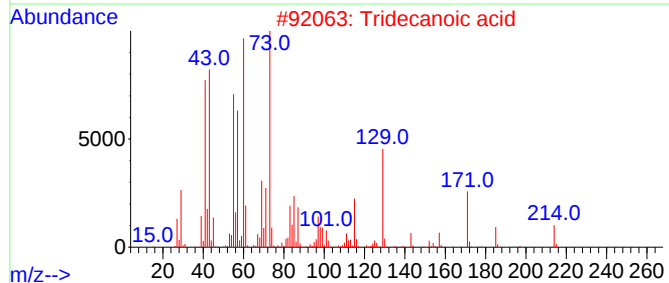
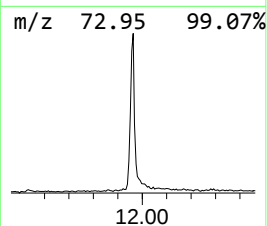
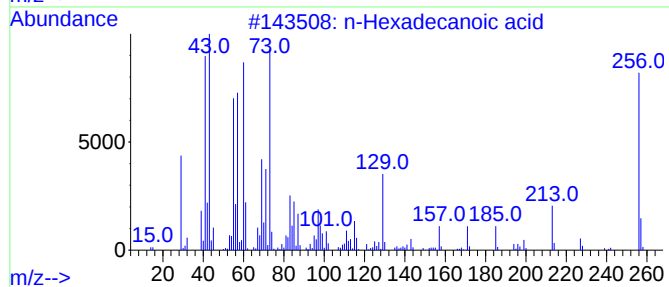
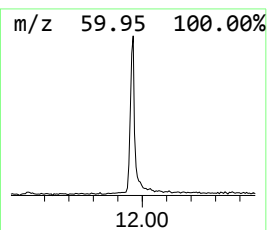
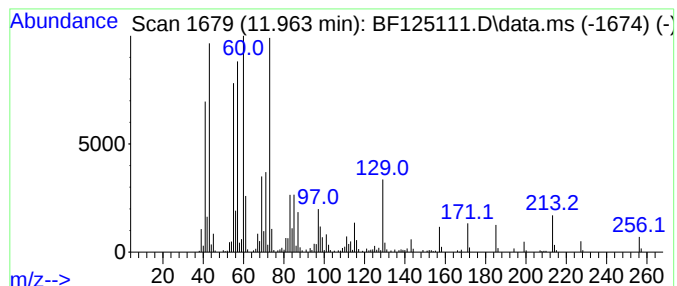
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	9.70 ng	737559	Phenanthrene-d10	11.445

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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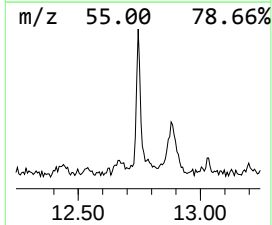
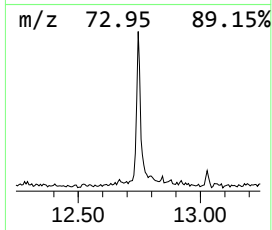
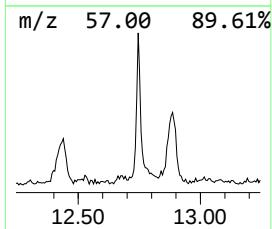
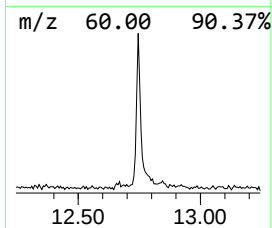
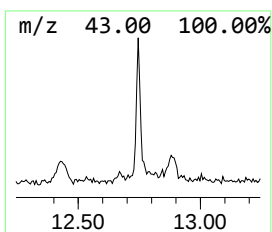
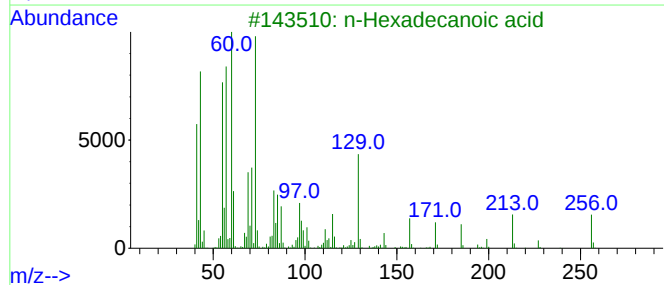
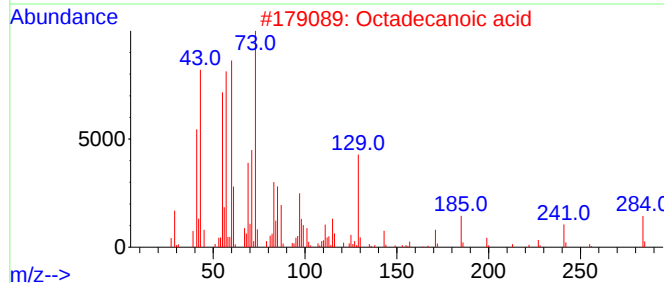
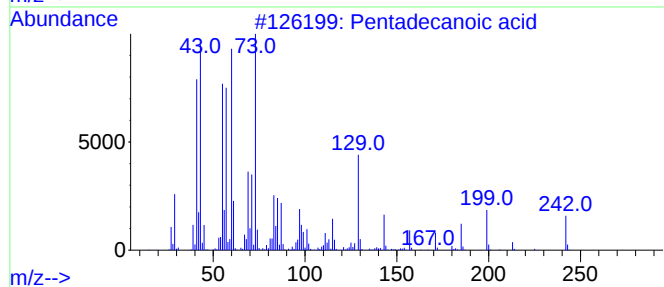
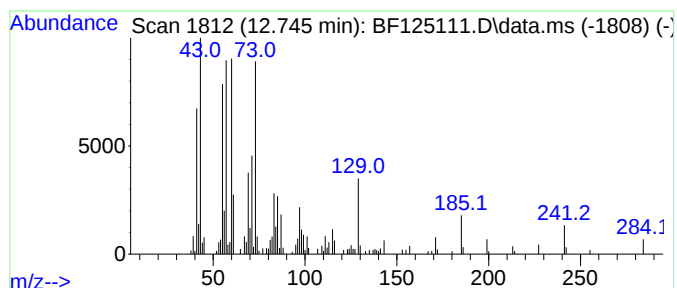
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Peak Number 5 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.745	4.30 ng	326988	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
2			Octadecanoic acid	284	C18H36O2	000057-11-4	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Undecanoic acid	186	C11H22O2	000112-37-8	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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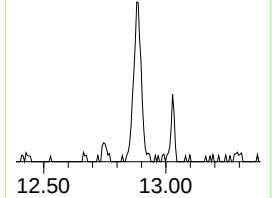
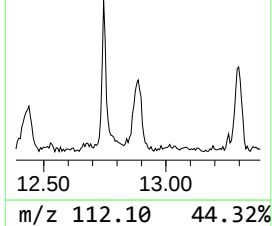
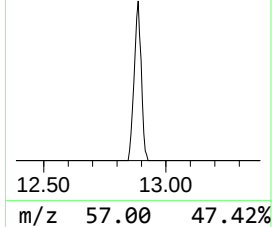
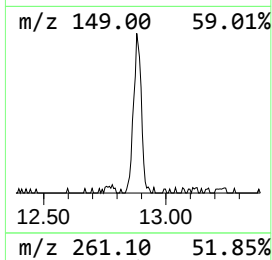
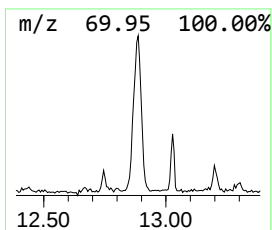
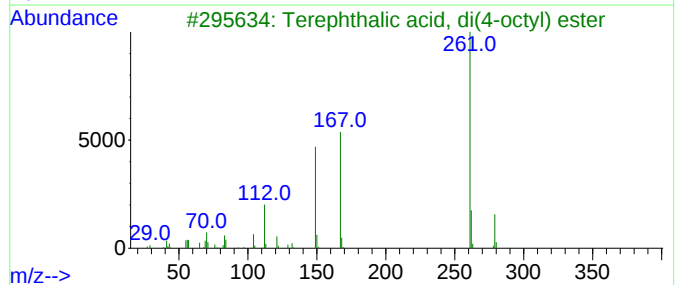
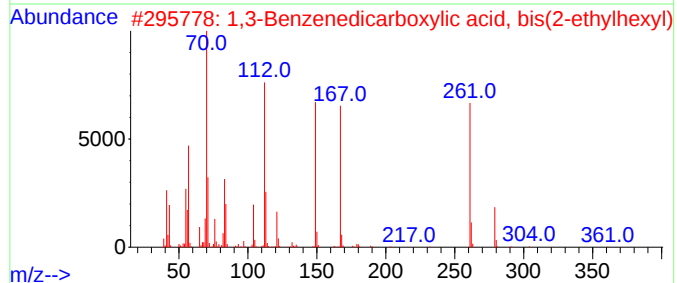
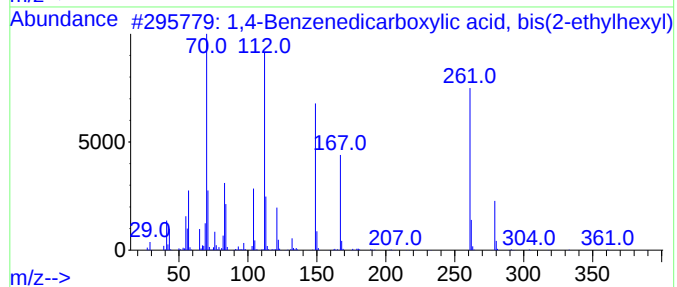
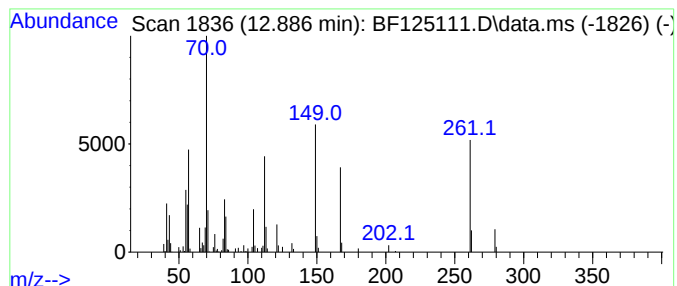
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	6.00 ng	351110	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	62
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
3			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38
4			Terephthalic acid, 1-cyclopentyl...	374	C23H34O4	1010323-84-1	35
5			Mono(2-ethylhexyl) phthalate	278	C16H22O4	004376-20-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125111.D
Acq On : 19 Aug 2021 13:22
Operator : JU/CG
Sample : M3442-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
210812088-01

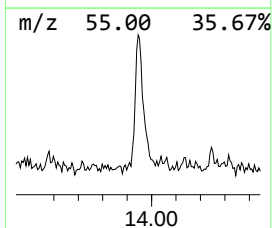
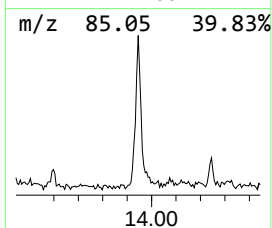
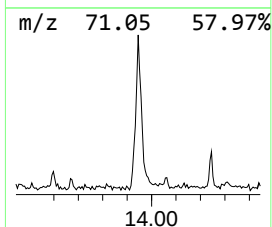
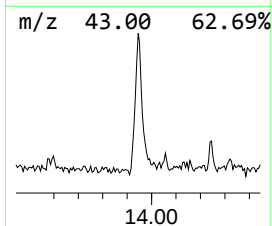
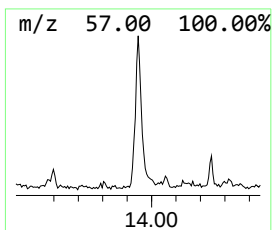
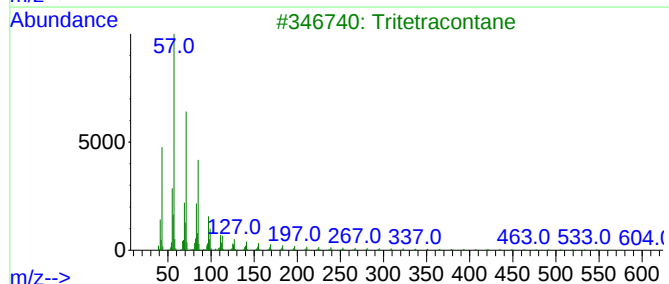
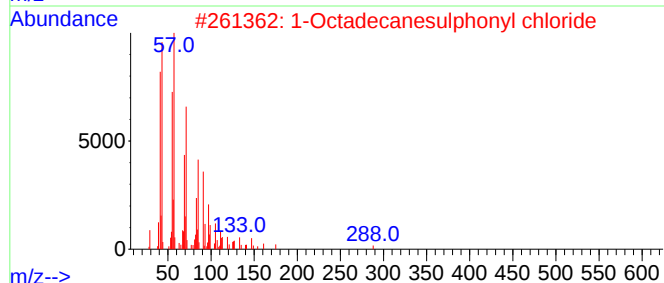
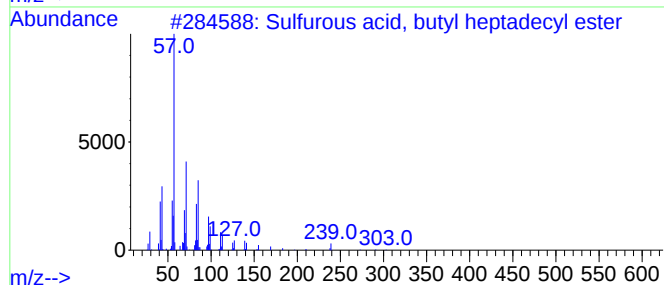
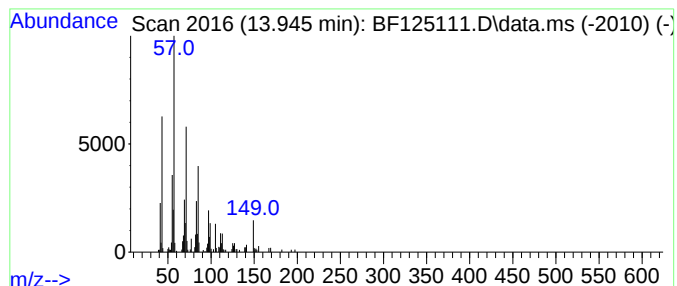
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl hepta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	5.74 ng	335846	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
2			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
3			Tritetracontane	605	C43H88	007098-21-7	90
4			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	90
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125111.D
Acq On : 19 Aug 2021 13:22
Operator : JU/CG
Sample : M3442-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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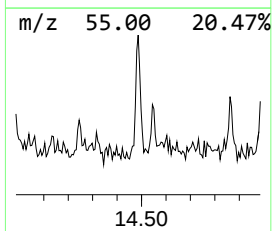
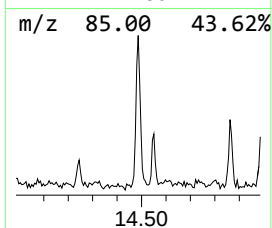
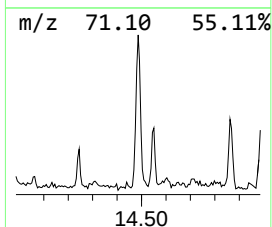
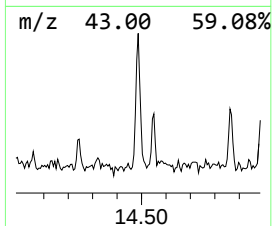
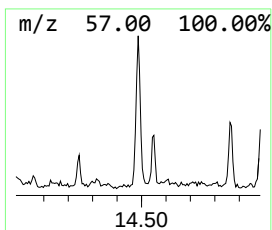
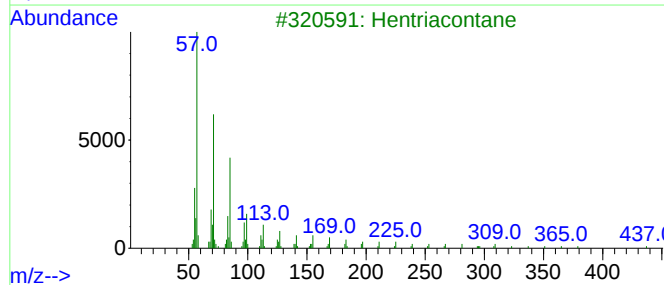
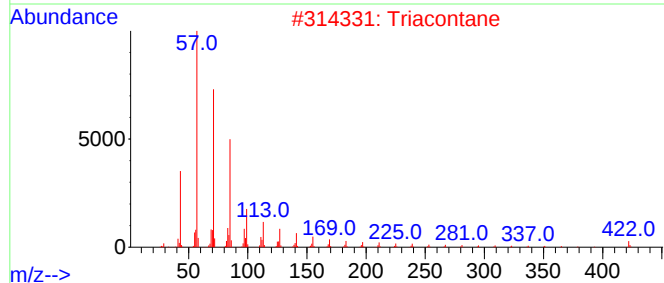
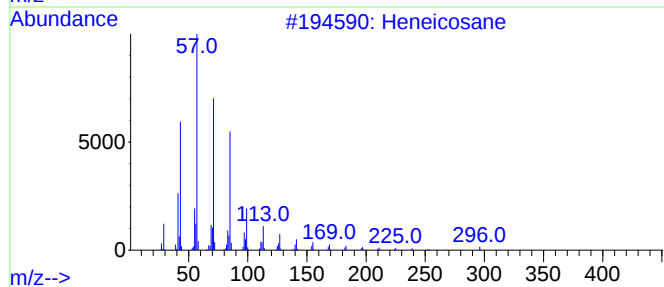
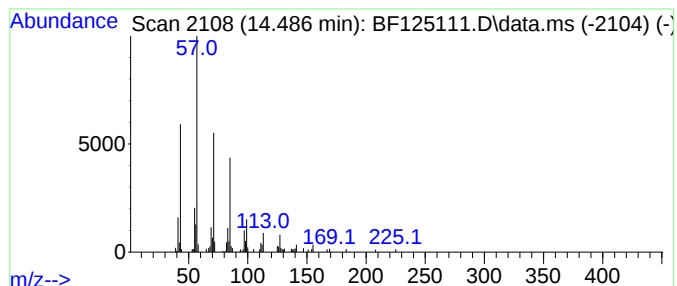
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	2.64 ng	154530	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Triacontane	422	C30H62	000638-68-6	90
3			Hentriacontane	437	C31H64	000630-04-6	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125111.D
Acq On : 19 Aug 2021 13:22
Operator : JU/CG
Sample : M3442-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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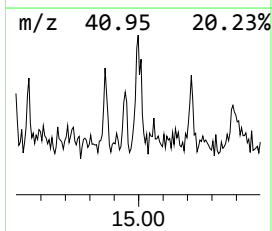
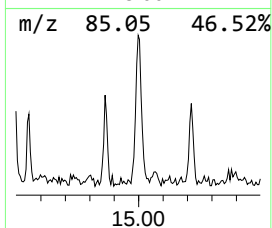
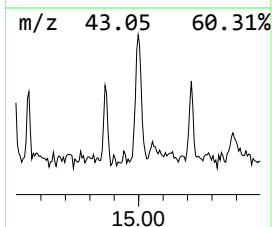
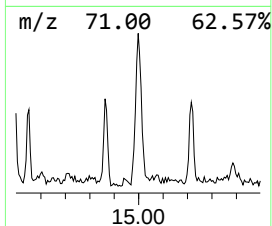
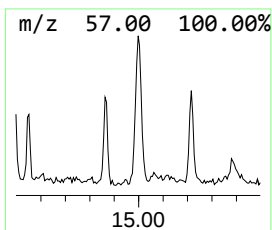
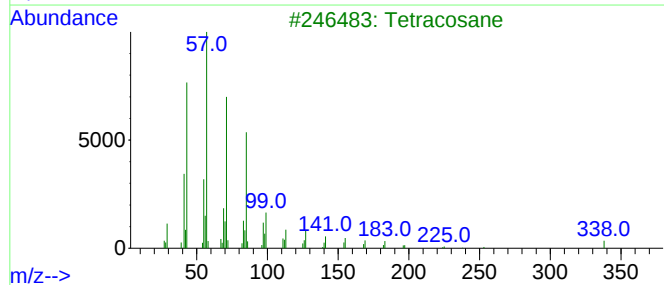
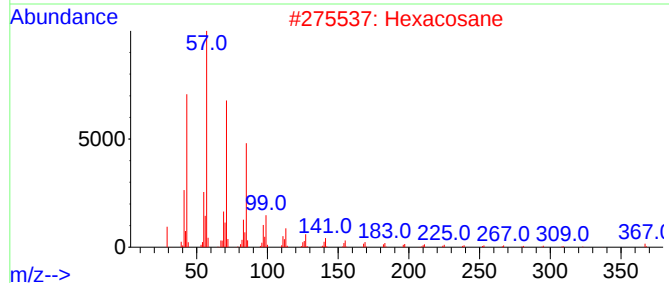
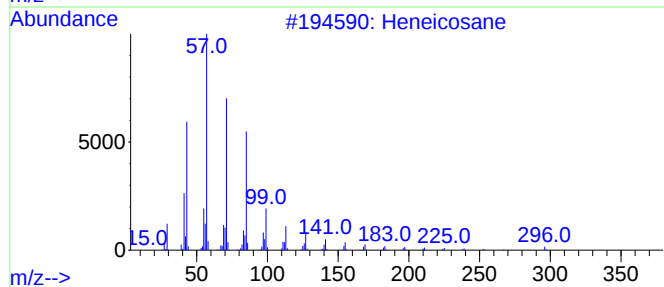
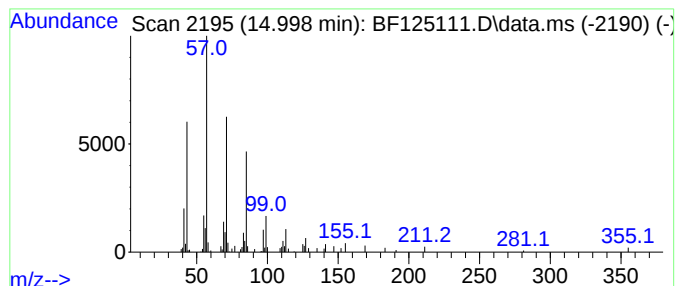
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	2.52 ng	147344	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Tetracosane	338	C24H50	000646-31-1	90
4			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125111.D
Acq On : 19 Aug 2021 13:22
Operator : JU/CG
Sample : M3442-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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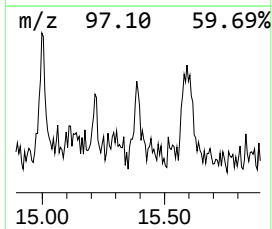
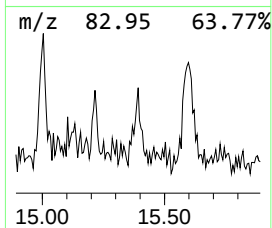
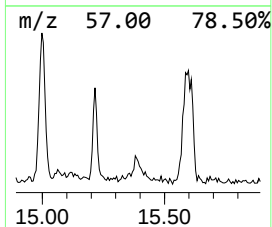
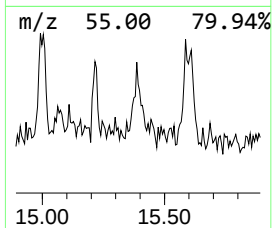
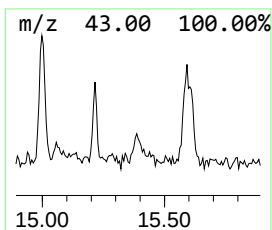
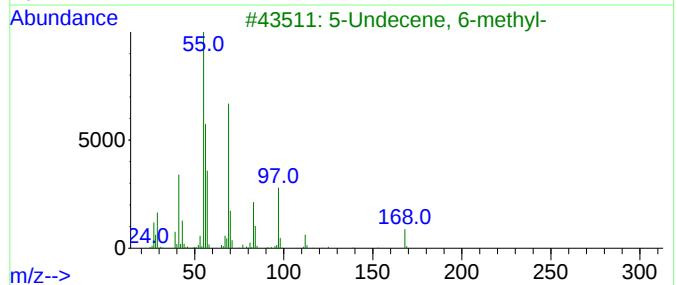
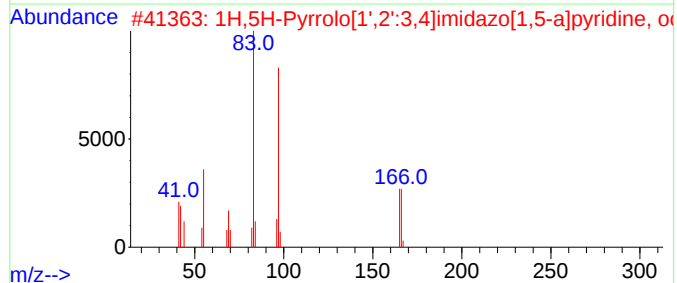
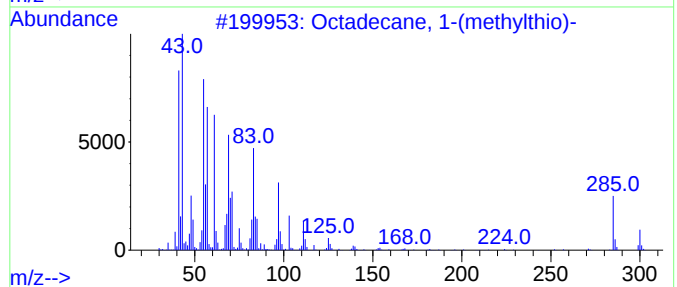
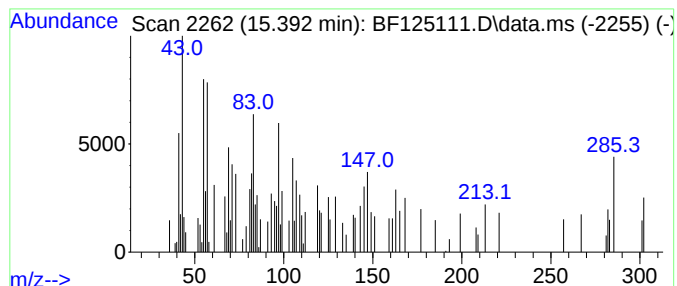
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.392 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	2.06 ng	120123	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-(methylthio)-	300	C19H40S	040289-98-3	12
2			1H,5H-Pyrrolo[1',2':3,4]imidazo[...	166	C10H18N2	054966-11-9	10
3			5-Undecene, 6-methyl-	168	C12H24	083687-45-0	10
4			2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	10
5			2-Thiopheneacetic acid, 6-ethyl-...	282	C16H26O2S	1000278-92-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125111.D
Acq On : 19 Aug 2021 13:22
Operator : JU/CG
Sample : M3442-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
210812088-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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-...	5.128	6.8	ng	343300	1	6.916	1004590	20.0
Ethanol, 2-(2-b...	8.098	7.9	ng	518386	2	8.198	1312990	20.0
n-Hexadecanoic ...	11.963	9.7	ng	737559	4	11.445	1521270	20.0
Pentadecanoic acid	12.745	4.3	ng	326988	4	11.445	1521270	20.0
1,4-Benzenedica...	12.886	6.0	ng	351110	5	14.080	1170460	20.0
Sulfurous acid,...	13.945	5.7	ng	335846	5	14.080	1170460	20.0
Triacontane	14.486	2.6	ng	154530	5	14.080	1170460	20.0
Heneicosane	14.998	2.5	ng	147344	6	15.580	1168320	20.0
unknown15.392	15.392	2.1	ng	120123	6	15.580	1168320	20.0