LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125120.D
Acq On : 19 Aug 2021 18:18
Operator : JU/CG
Sample : M3430-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-1

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: BF125120.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	17	23	29	rVB	1444435	1841570	41.76%	5.525%
2	5.151	512	521	527	rVB	108074	140323	3.18%	0.421%
3	5.534	581	586	589	rBV	3920570	4096245	92.88%	12.290%
4	6.540	751	757	760	rBV	3655430	4136970	93.80%	12.413%
5	6.916	818	821	825	rVB	1230223	1045042	23.70%	3.136%
6	7.481	912	917	920	rBV	2948986	2693350	61.07%	8.081%
7	8.098	1018	1022	1025	rBV	1295407	1004779	22.78%	3.015%
8	8.198	1035	1039	1043	rVB	1576467	1349878	30.61%	4.050%
9	9.281	1217	1223	1226	rBV	4608122	4410325	100.00%	13.233%
10	9.957	1334	1338	1341	rBV	1847500	1456419	33.02%	4.370%
11	10.745	1467	1472	1475	rBV	3157177	2766496	62.73%	8.301%
12	11.445	1587	1591	1593	rBV	1543537	1431899	32.47%	4.296%
13	11.463	1593	1594	1598	rVB	76764	49135	1.11%	0.147%
14	11.957	1673	1678	1683	rBV2	167408	201394	4.57%	0.604%
15	12.651	1793	1796	1800	rBV	124337	116600	2.64%	0.350%
16	12.745	1809	1812	1819	rBV3	53832	59310	1.34%	0.178%
17	12.880	1831	1835	1841	rBV	112558	122790	2.78%	0.368%
18	13.033	1856	1861	1864	rBV	3853757	3816613	86.54%	11.451%
19	13.927	2009	2013	2027	rBV3	122656	338349	7.67%	1.015%
20	14.080	2034	2039	2042	rBV	1063887	1000152	22.68%	3.001%
21	14.104	2042	2043	2050	rVB	55256	47803	1.08%	0.143%
22	15.133	2214	2218	2226	rVB2	50686	101941	2.31%	0.306%
23	15.510	2278	2282	2287	rVB	45476	57990	1.31%	0.174%
24	15.580	2288	2294	2298	rVV	746880	953240	21.61%	2.860%
25	15.610	2298	2299	2306	rVB5	46513	46036	1.04%	0.138%
26	16.062	2373	2376	2382	rVB2	30157	44282	1.00%	0.133%

Sum of corrected areas: 33328931

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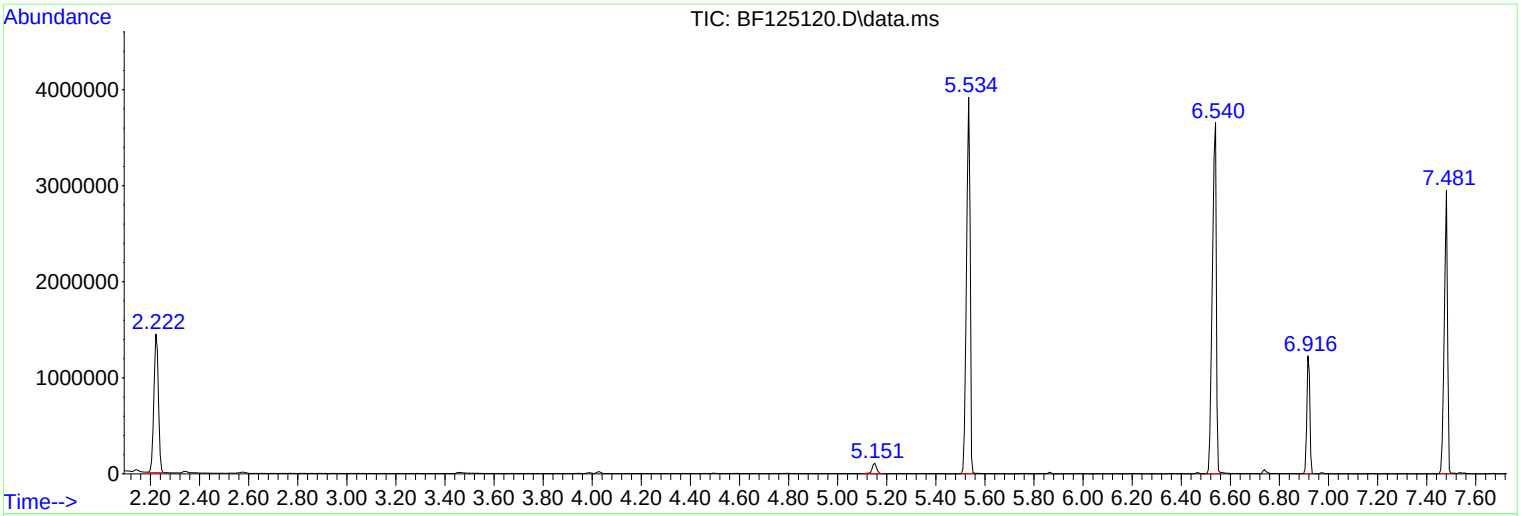
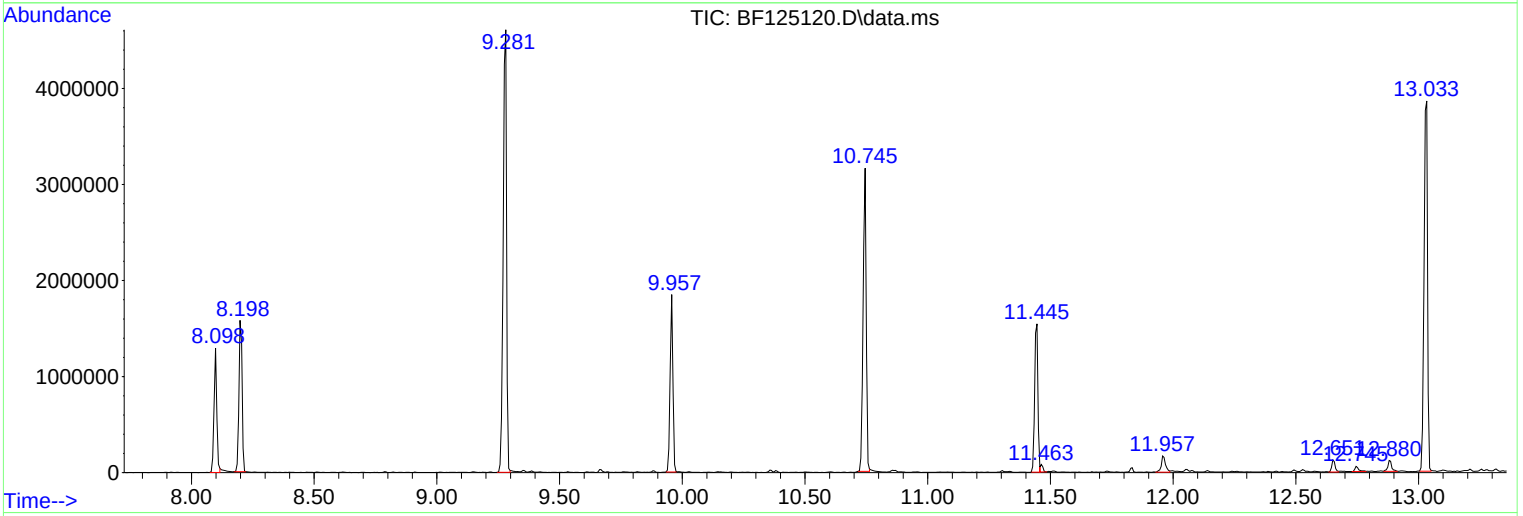
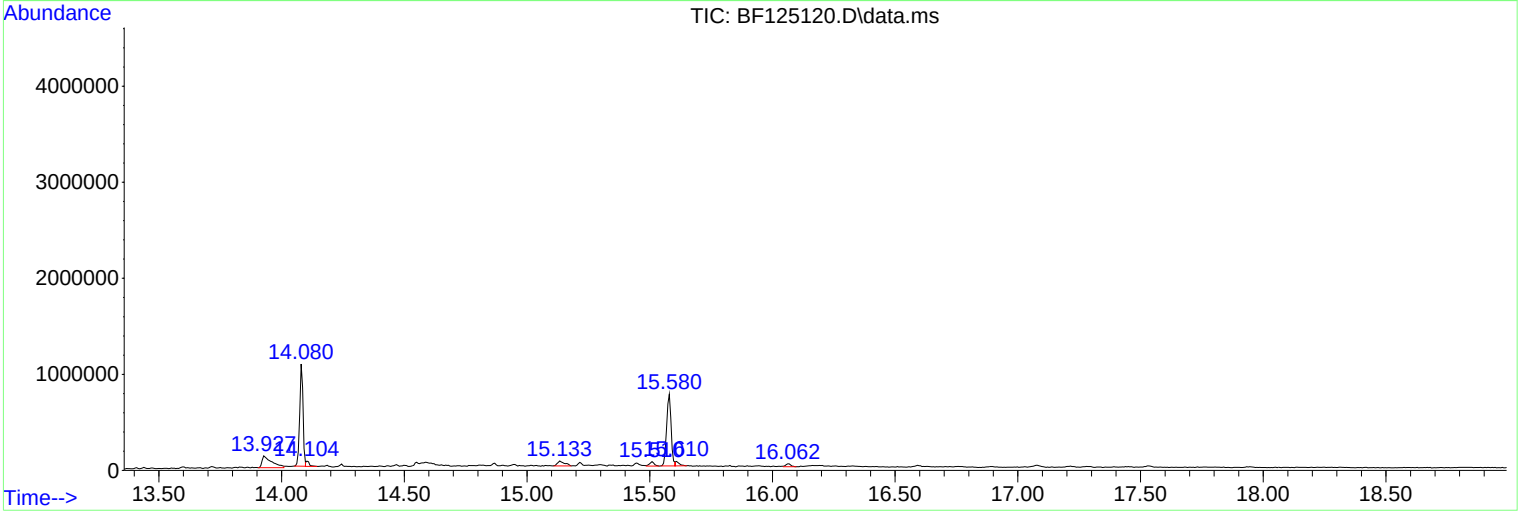
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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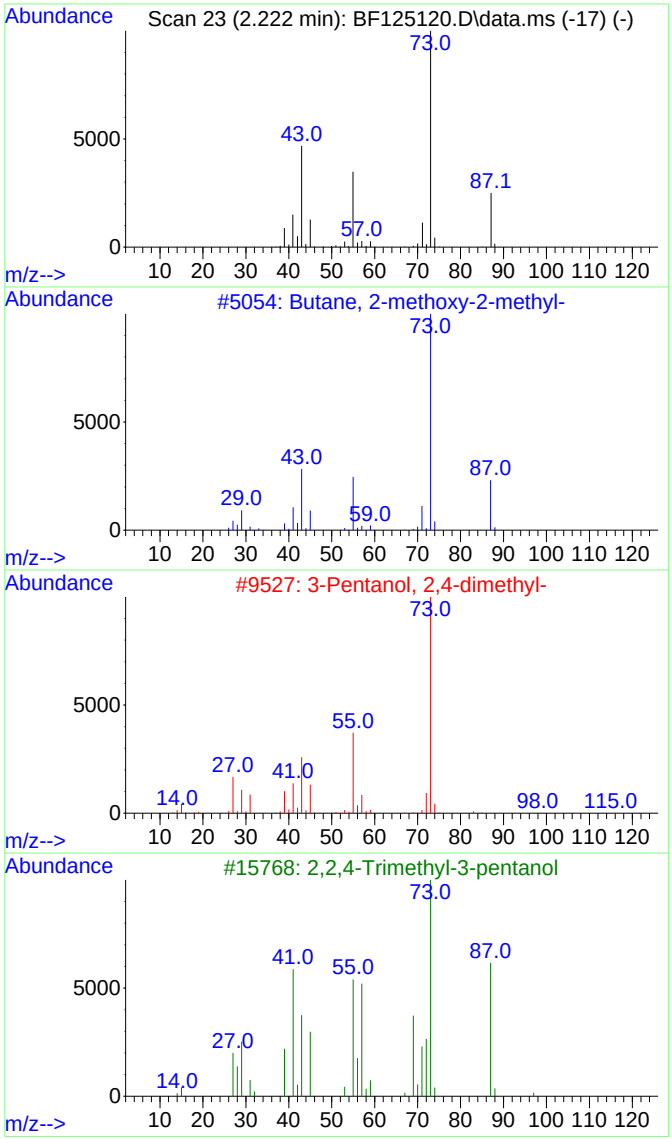
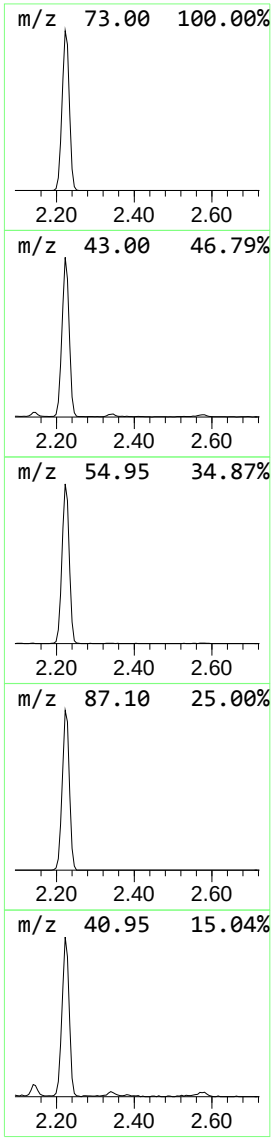
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	35.24 ng	1841570	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	39
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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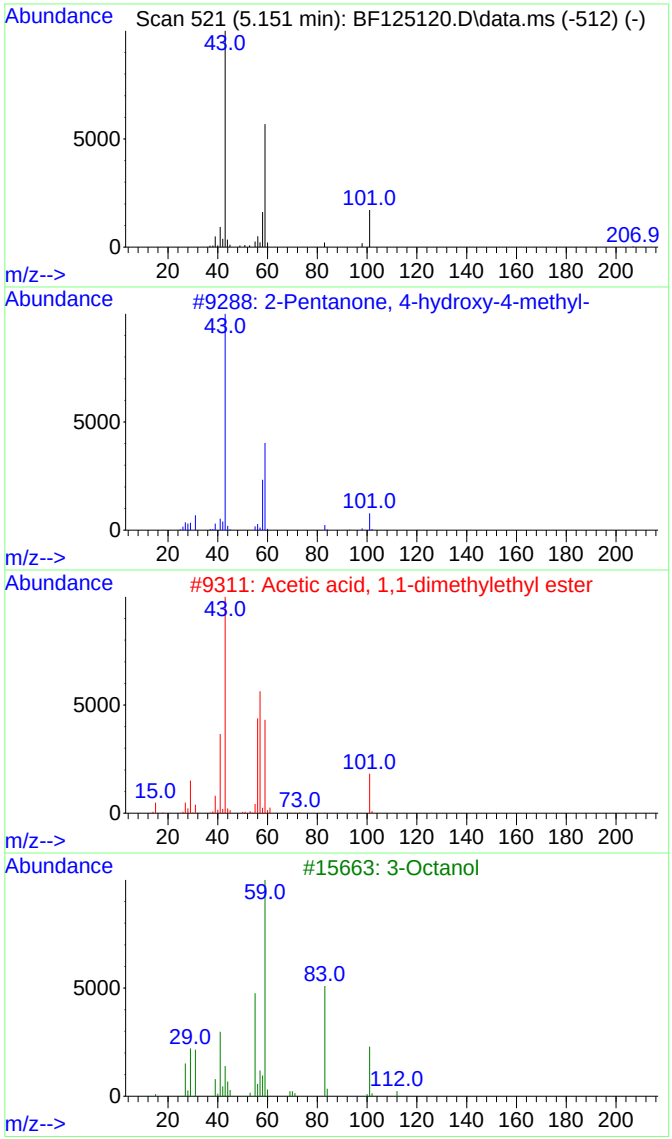
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

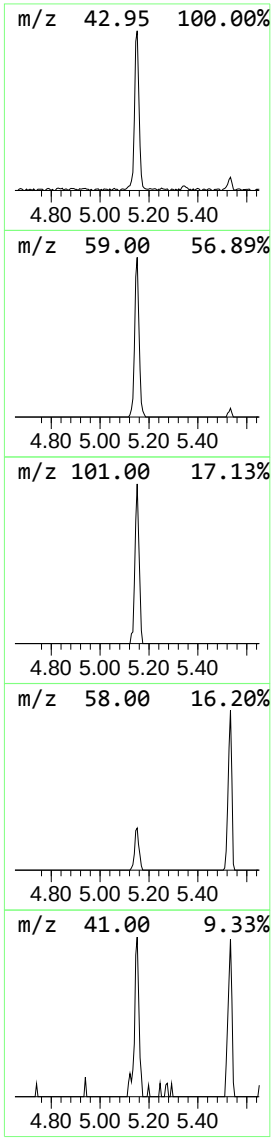
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	2.69 ng	140323	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Octanol	130	C8H18O	000589-98-0	36
4	3-Hexanol	102	C6H14O	000623-37-0	36
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33





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Sample : M3430-01
Misc :
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Instrument : BNA_F
ClientSampleId : PE-1

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TIC Library : C:\Database\NIST20.L
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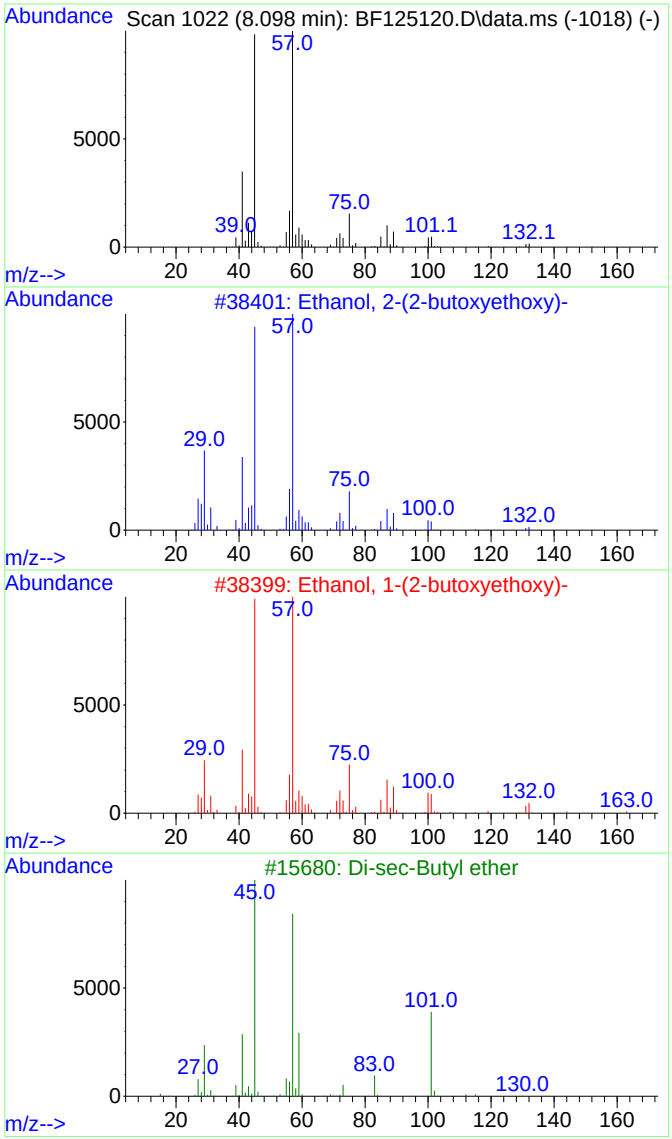
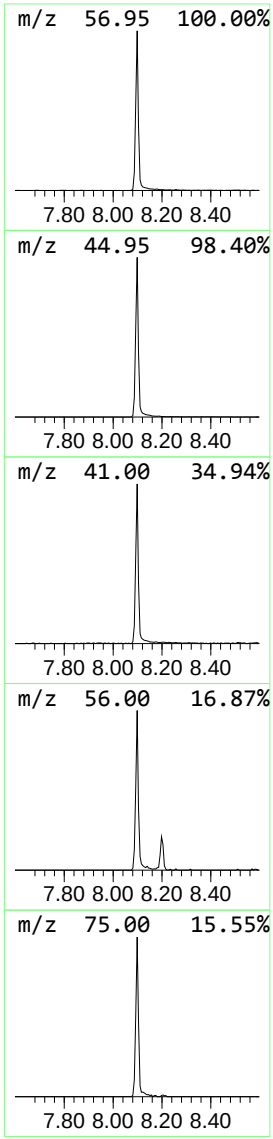
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	14.89 ng	1004780	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	90
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50





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Instrument : BNA_F
ClientSampleId : PE-1

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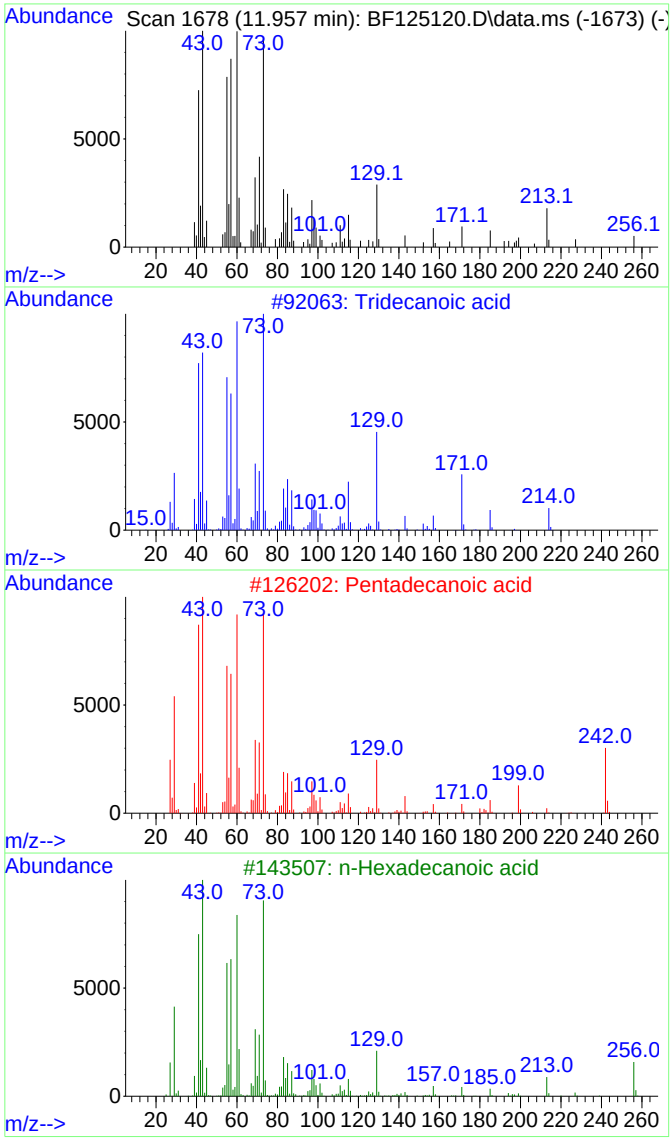
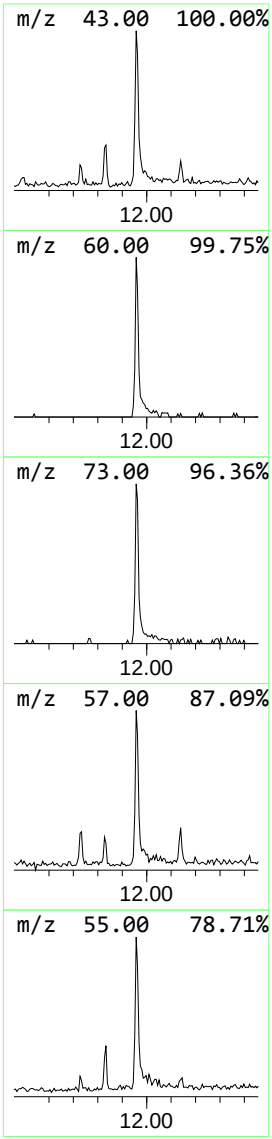
Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	2.81 ng	201394	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	25





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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-1

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
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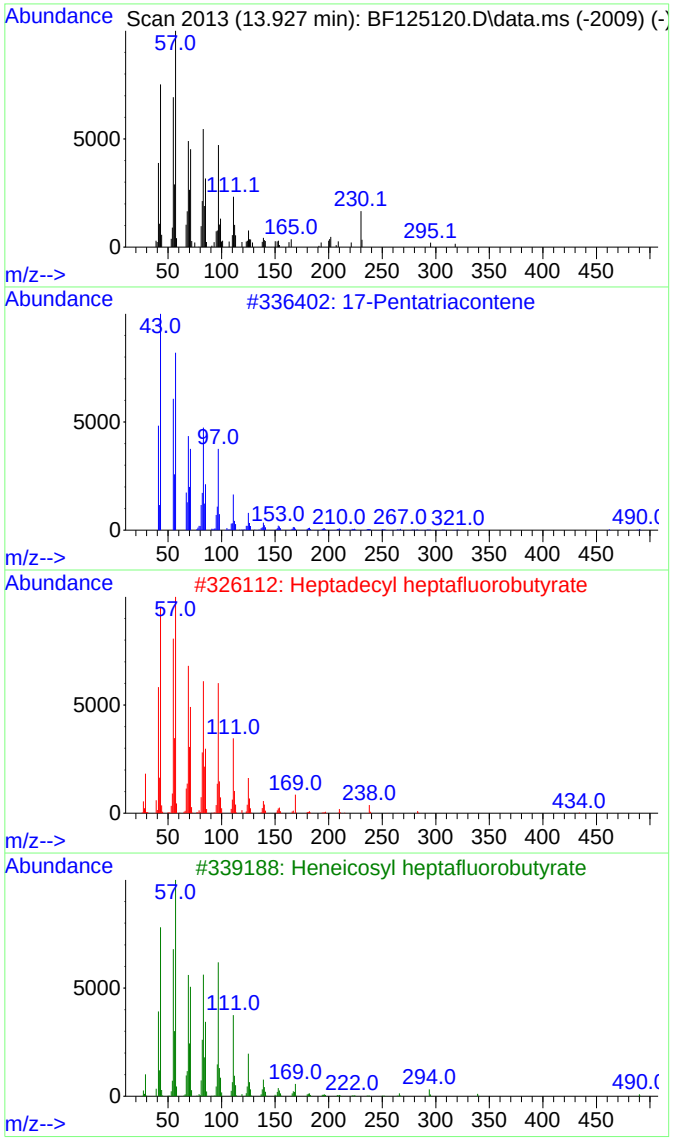
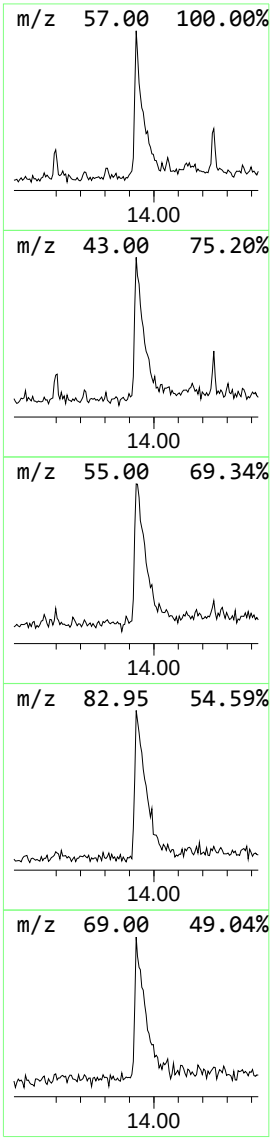
Peak Number 6 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	6.77 ng	338349	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	90
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
5	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	87





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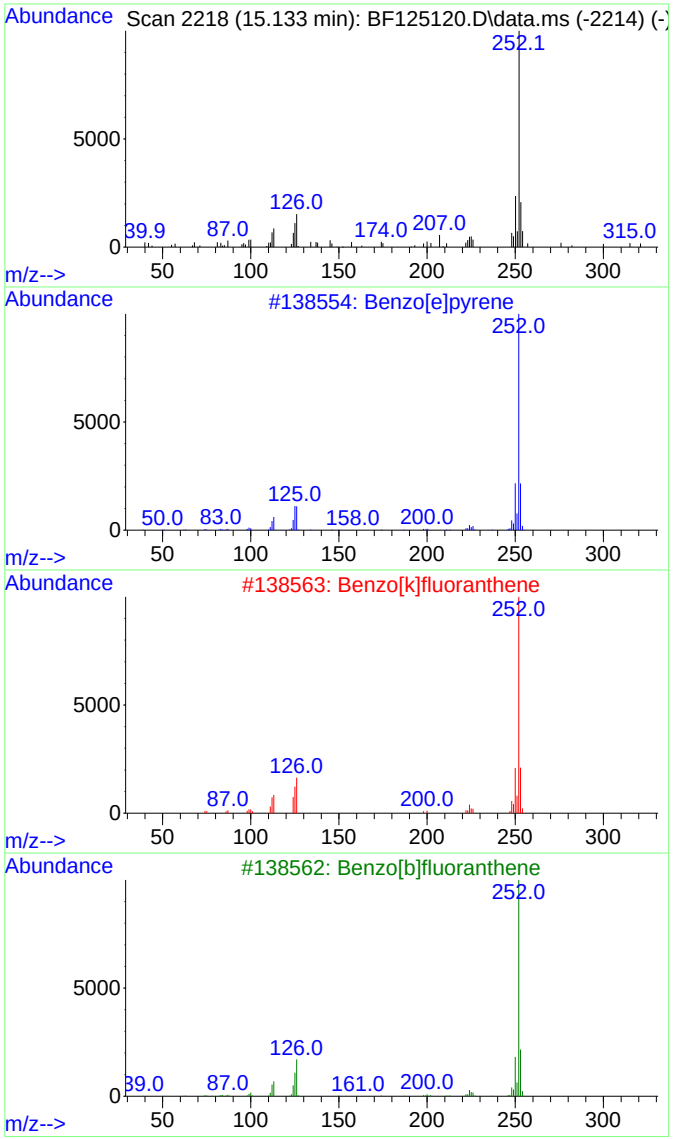
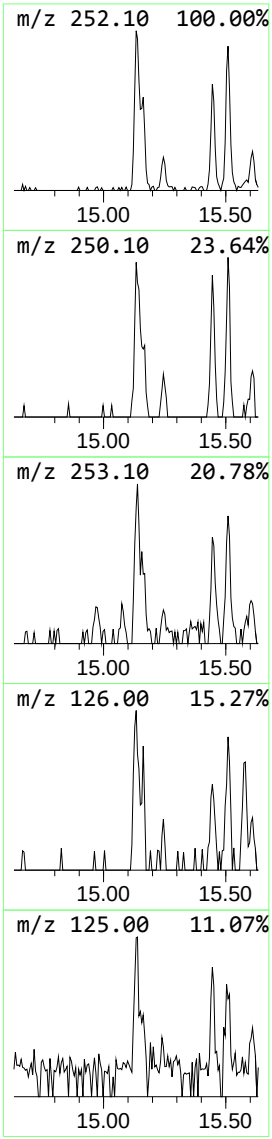
Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	2.14 ng	101941	Perylene-d12	15.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.222	35.2	ng	1841570	1	6.916	1045040	20.0
2-Pentanone, 4-...	5.151	2.7	ng	140323	1	6.916	1045040	20.0
Ethanol, 2-(2-b...	8.098	14.9	ng	1004780	2	8.198	1349880	20.0
Tridecanoic acid	11.957	2.8	ng	201394	4	11.445	1431900	20.0
17-Pentatriacon...	13.927	6.8	ng	338349	5	14.080	1000150	20.0
Benzo[e]pyrene	15.133	2.1	ng	101941	6	15.580	953240	20.0