LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126092.D
Acq On : 9 Nov 2021 20:57
Operator : JU/CG
Sample : M4582-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VWE-B10-110621-0-10

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126092.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	3	12	17	rBV	1927409	2436775	37.94%	5.938%
2	2.263	25	30	37	rBV	72574	97621	1.52%	0.238%
3	5.075	504	508	516	rVB	261666	323683	5.04%	0.789%
4	5.475	570	576	579	rBV	5065934	4794282	74.64%	11.683%
5	6.481	741	747	750	rBV	4802658	5009912	78.00%	12.208%
6	6.851	806	810	813	rBV	1549052	1178480	18.35%	2.872%
7	7.416	900	906	909	rBV	3436880	3353519	52.21%	8.172%
8	8.033	1007	1011	1024	rBV	1184958	1242116	19.34%	3.027%
9	8.133	1024	1028	1031	rBV	1874201	1479295	23.03%	3.605%
10	9.210	1206	1211	1214	rBV	7663931	6423304	100.00%	15.652%
11	9.886	1322	1326	1329	rBV	2211153	1732168	26.97%	4.221%
12	10.674	1455	1460	1463	rBV	4164860	3640321	56.67%	8.871%
13	11.369	1574	1578	1581	rBV	1861171	1532803	23.86%	3.735%
14	11.763	1642	1645	1649	rBV	161637	142237	2.21%	0.347%
15	12.468	1763	1765	1769	rVB	128046	105164	1.64%	0.256%
16	12.957	1844	1848	1851	rBV	5808136	4651454	72.42%	11.335%
17	13.857	1998	2001	2012	rVB	317434	432591	6.73%	1.054%
18	14.004	2022	2026	2030	rBV	1077034	1008532	15.70%	2.458%
19	14.498	2105	2110	2114	rBV4	67771	131614	2.05%	0.321%
20	14.868	2170	2173	2176	rBV	100277	89329	1.39%	0.218%
21	14.974	2188	2191	2199	rVB10	56054	94100	1.46%	0.229%
22	15.474	2271	2276	2280	rBV	835793	1023901	15.94%	2.495%
23	16.015	2363	2368	2373	rBV8	56701	114276	1.78%	0.278%

Sum of corrected areas: 41037477

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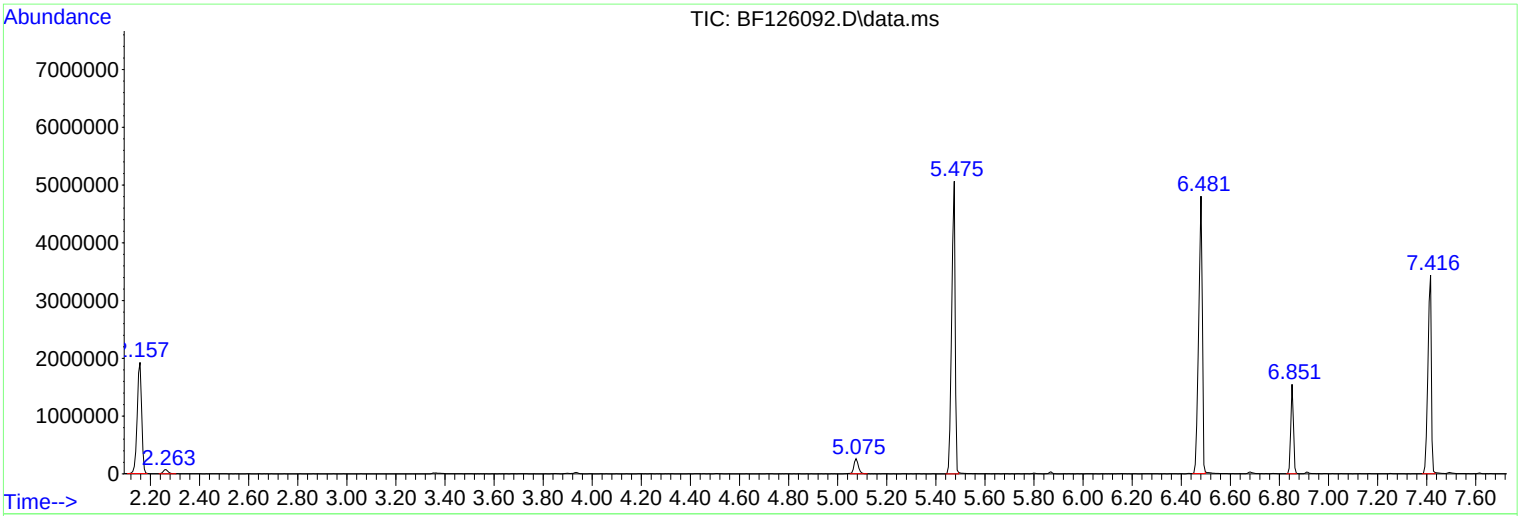
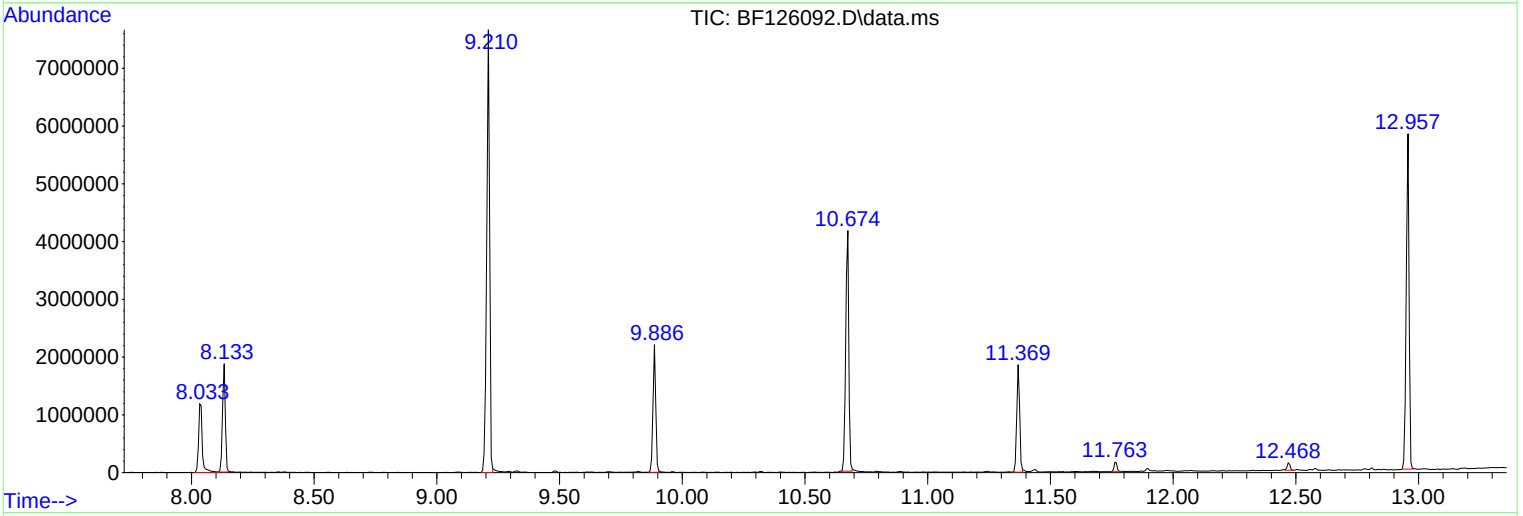
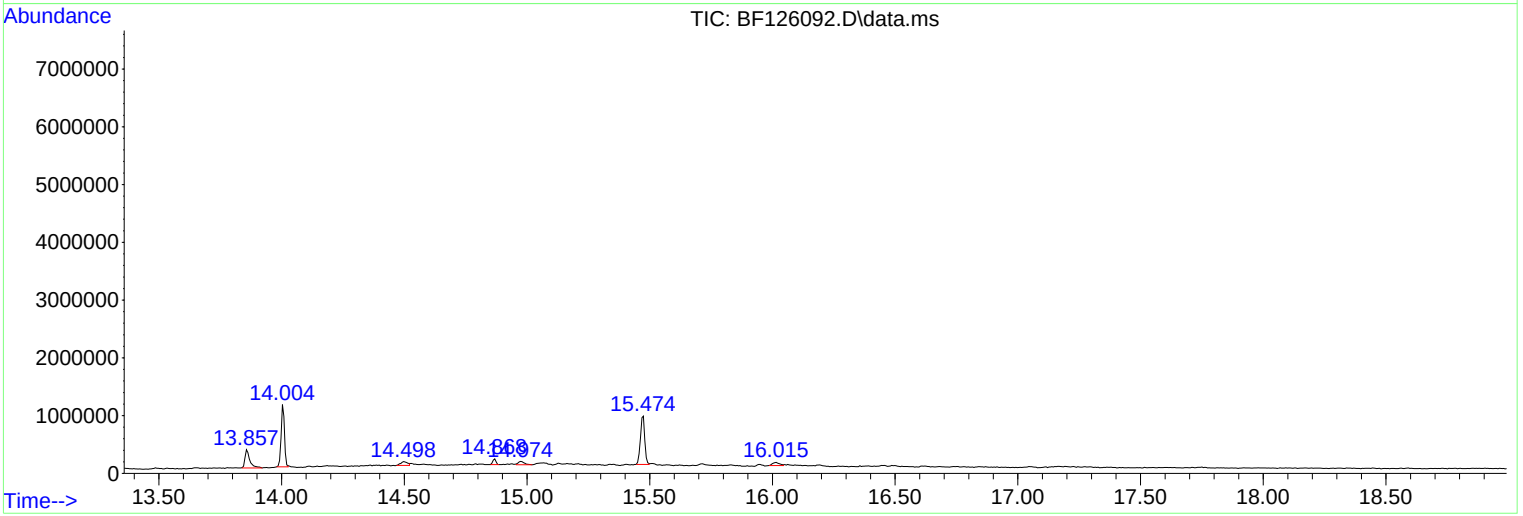
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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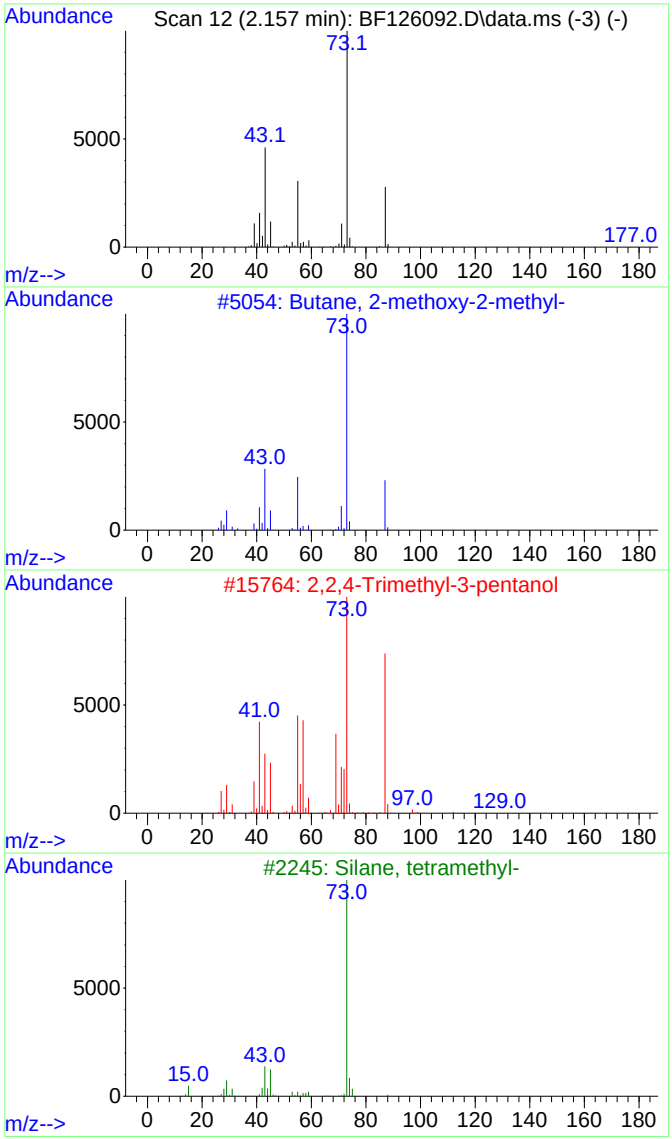
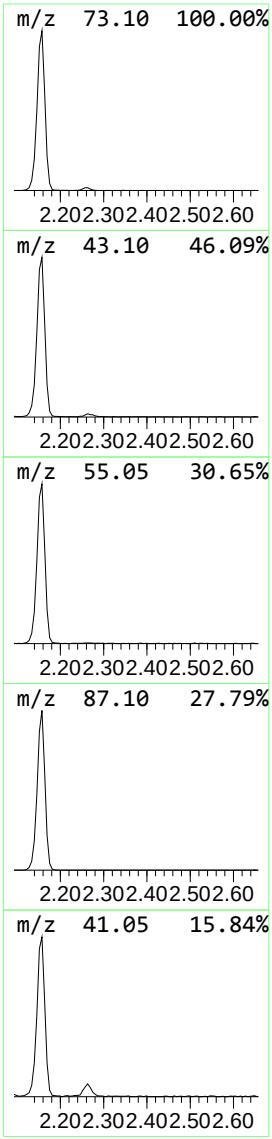
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	41.35 ng	2436780	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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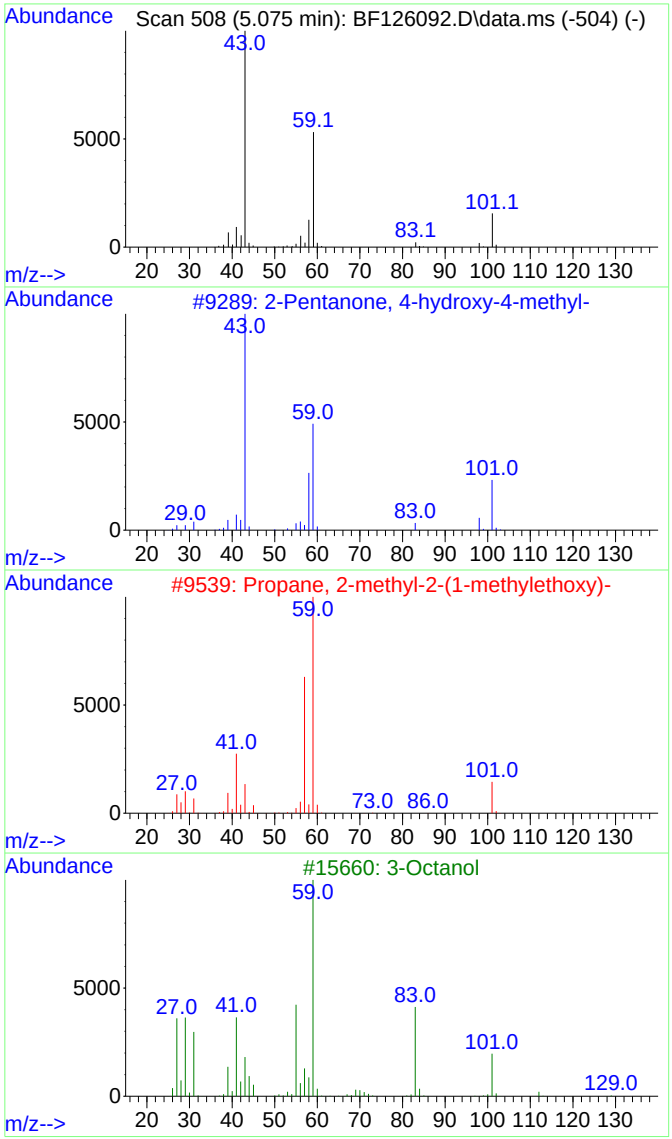
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

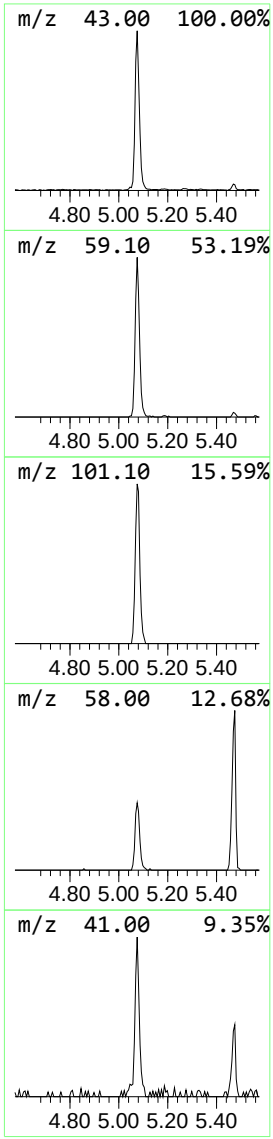
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.49 ng	323683	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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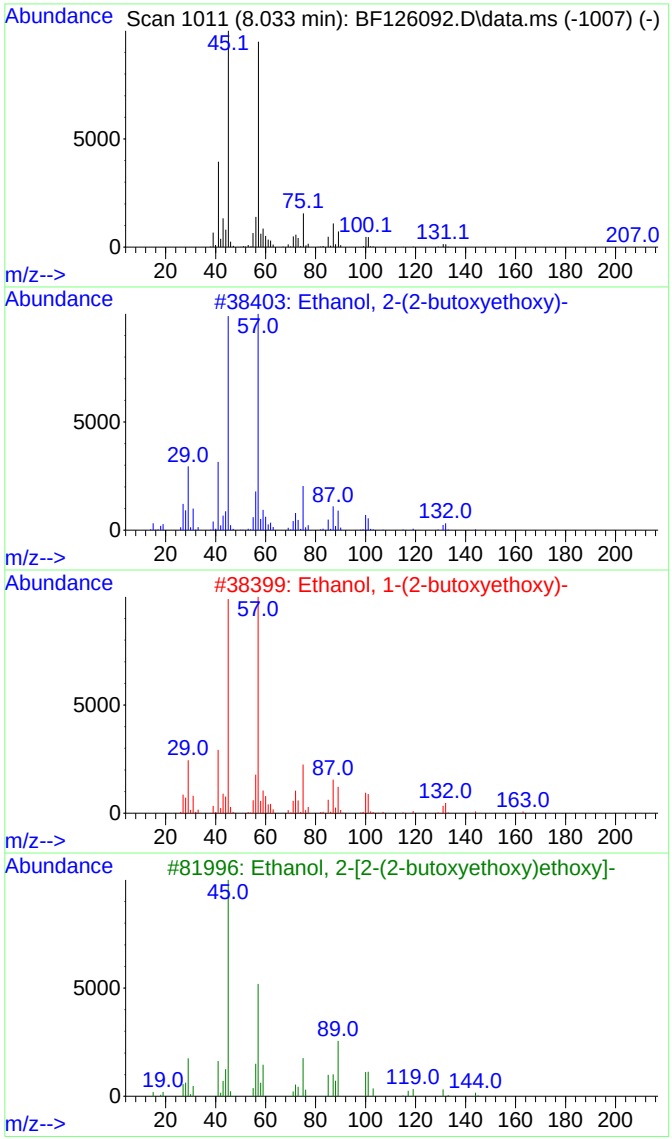
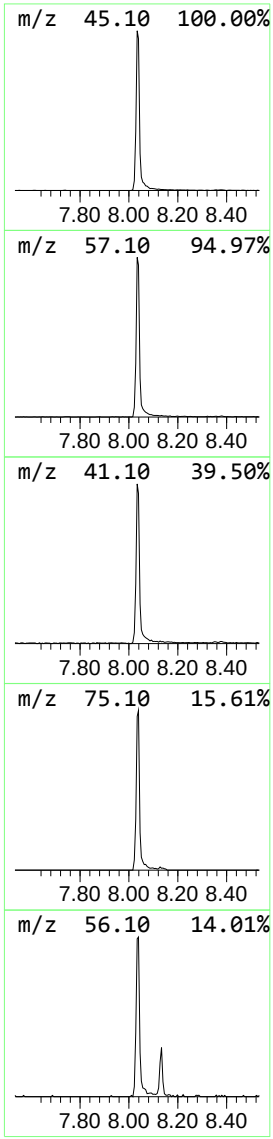
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.033	16.79 ng	1242120	Naphthalene-d8	8.133

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	83
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	72
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53





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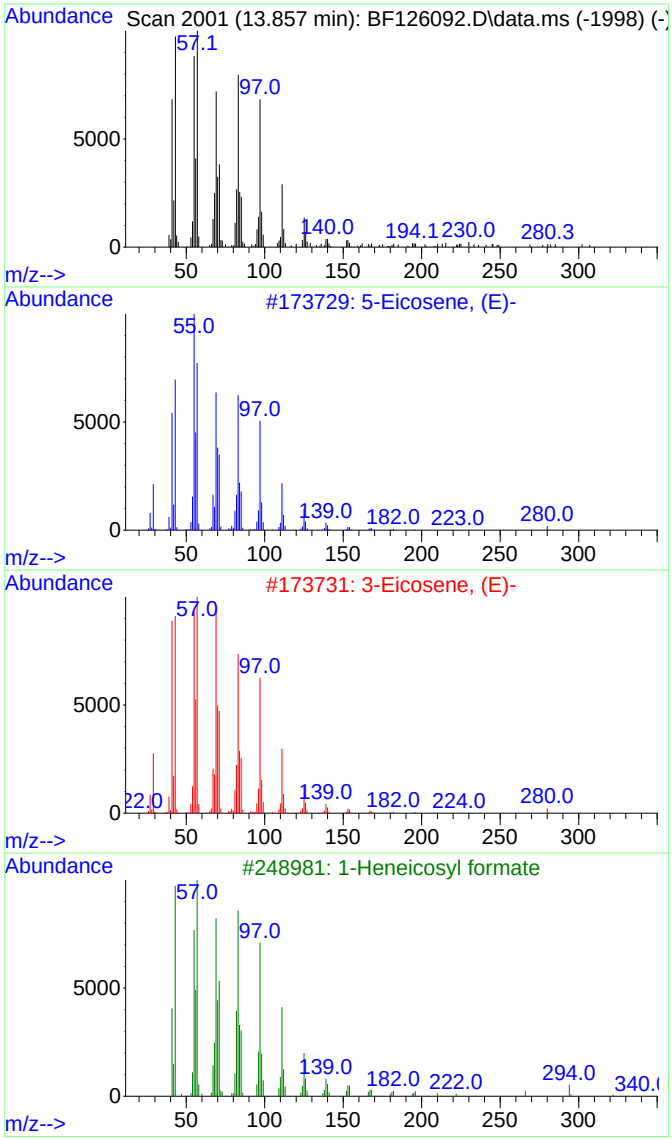
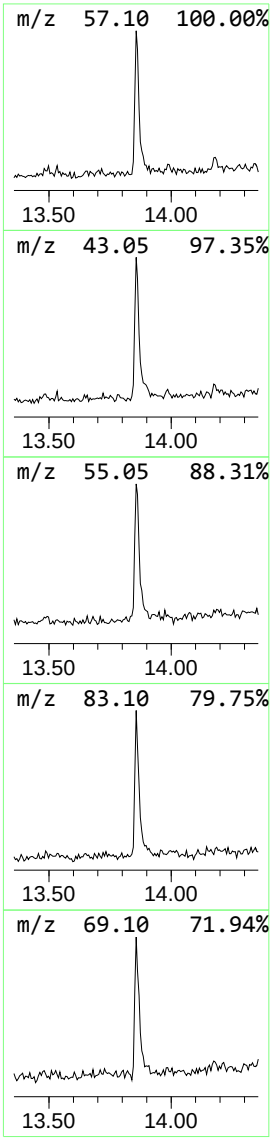
****

Peak Number 4 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	8.58 ng	432591	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
4	1-Docosene	308	C22H44	001599-67-3	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





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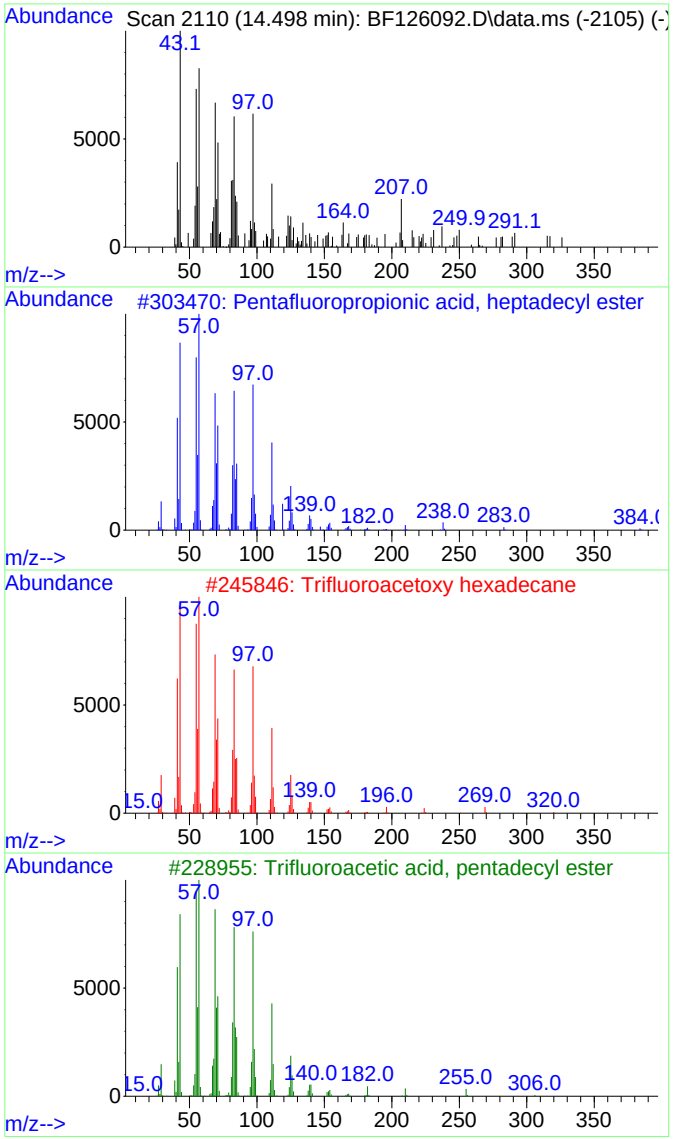
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

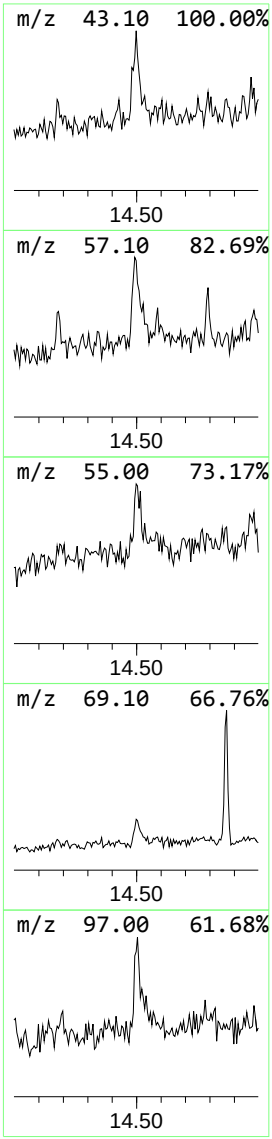
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	2.61 ng	131614	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	81
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	70
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	70
4	Triacontan-15-ol	438	C30H62O	031849-26-0	68
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64





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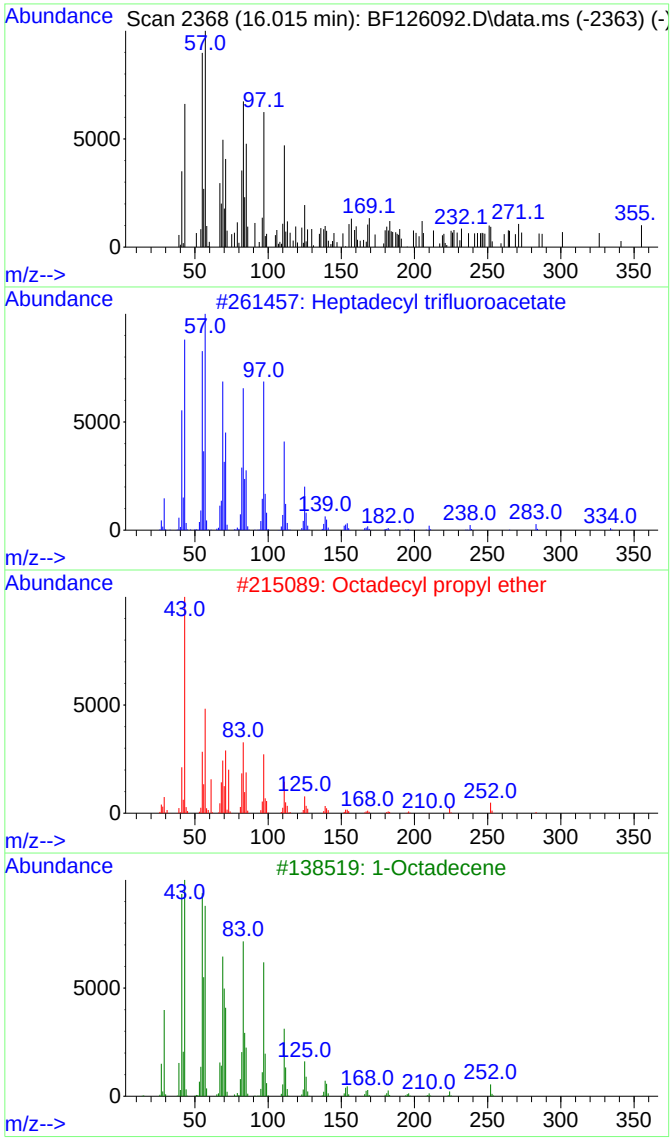
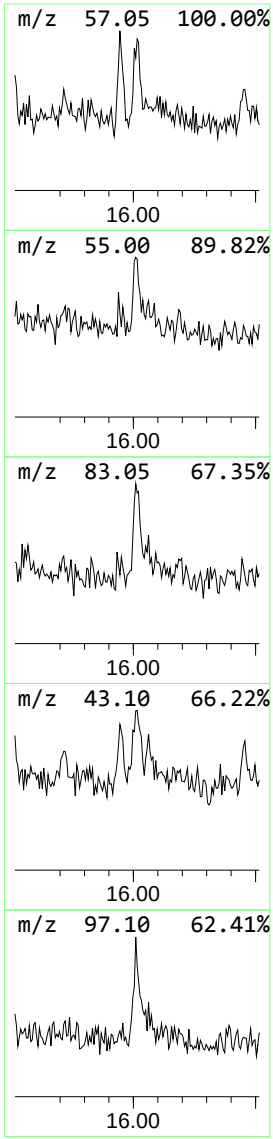
****

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	2.23 ng	114276	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	74
2	Octadecyl propyl ether	312	C21H44O	1000406-28-0	72
3	1-Octadecene	252	C18H36	000112-88-9	70
4	1-Heptacosanol	396	C27H56O	002004-39-9	70
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	64





Tentatively Identified Compound (LSC) summary

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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...	2.157	41.4	ng	2436780	1	6.851	1178480	20.0
2-Pentanone, 4-...	5.075	5.5	ng	323683	1	6.851	1178480	20.0
Ethanol, 2-(2-b...	8.033	16.8	ng	1242120	2	8.133	1479300	20.0
5-Eicosene, (E)-	13.857	8.6	ng	432591	5	14.004	1008530	20.0
Pentafluoroprop...	14.498	2.6	ng	131614	5	14.004	1008530	20.0
Heptadecyl trif...	16.015	2.2	ng	114276	6	15.474	1023900	20.0