LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121024\
Data File : BF140814.D
Acq On : 10 Dec 2024 18:52
Operator : RC/JU
Sample : P5216-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-12

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-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140814.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	5	14	29	rVB	1574910	2684647	95.60%	14.130%
2	5.116	510	514	526	rVB	20022	33449	1.19%	0.176%
3	5.510	576	581	599	rBV	1559098	2063113	73.47%	10.859%
4	6.516	746	752	767	rBV	1549087	2178927	77.59%	11.468%
5	6.863	806	811	816	rBV	356642	448376	15.97%	2.360%
6	7.428	901	907	912	rBV	1054636	1432119	51.00%	7.538%
7	7.681	946	950	957	rVB	51448	69318	2.47%	0.365%
8	8.139	1023	1028	1035	rBV	428832	583419	20.78%	3.071%
9	8.298	1052	1055	1059	rVB	57736	75662	2.69%	0.398%
10	9.216	1204	1211	1216	rBV	2089764	2808229	100.00%	14.781%
11	9.898	1323	1327	1350	rVB2	762999	1585824	56.47%	8.347%
12	10.616	1444	1449	1454	rVB	134065	171556	6.11%	0.903%
13	10.692	1457	1462	1475	rVV	1022646	1370312	48.80%	7.212%
14	11.392	1576	1581	1588	rBV	412701	545702	19.43%	2.872%
15	11.910	1665	1669	1678	rBV	192343	278511	9.92%	1.466%
16	12.610	1785	1788	1794	rBV	31775	41560	1.48%	0.219%
17	12.698	1800	1803	1813	rVB3	28689	48602	1.73%	0.256%
18	12.974	1845	1850	1856	rBV	1358363	1769727	63.02%	9.315%
19	13.863	1997	2001	2013	rVB	121292	179038	6.38%	0.942%
20	14.039	2027	2031	2044	rVB	264302	401425	14.29%	2.113%
21	15.539	2282	2286	2294	rVB	142732	230031	8.19%	1.211%

Sum of corrected areas: 18999547

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Instrument :
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ClientSampleId :
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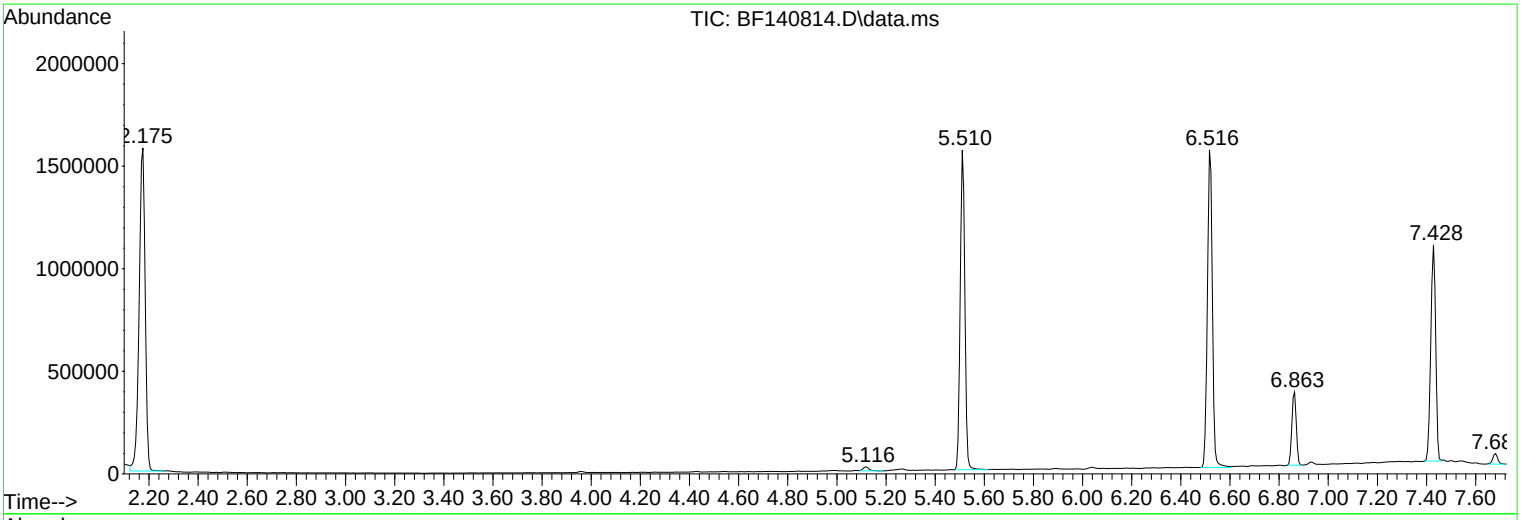
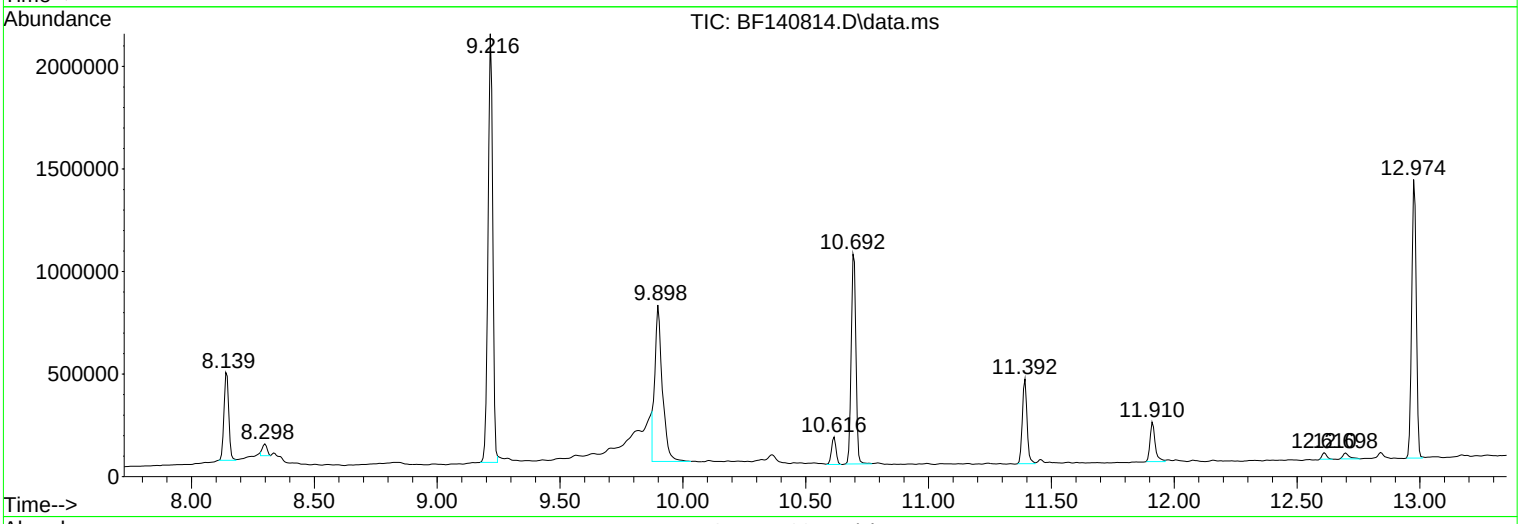
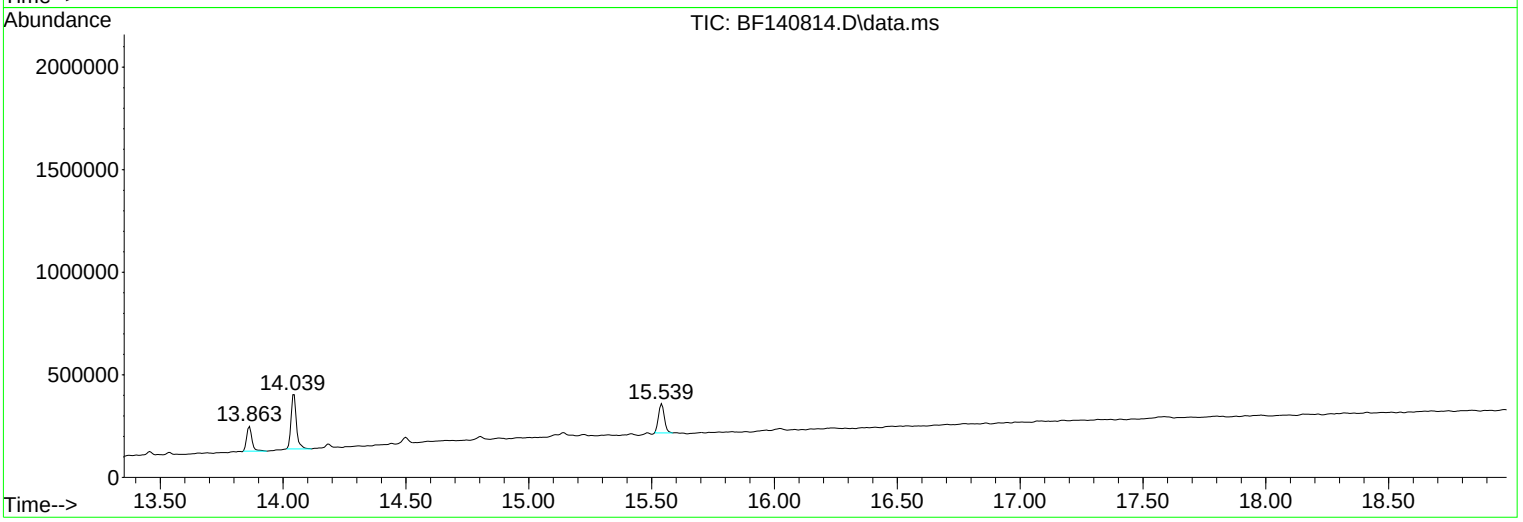
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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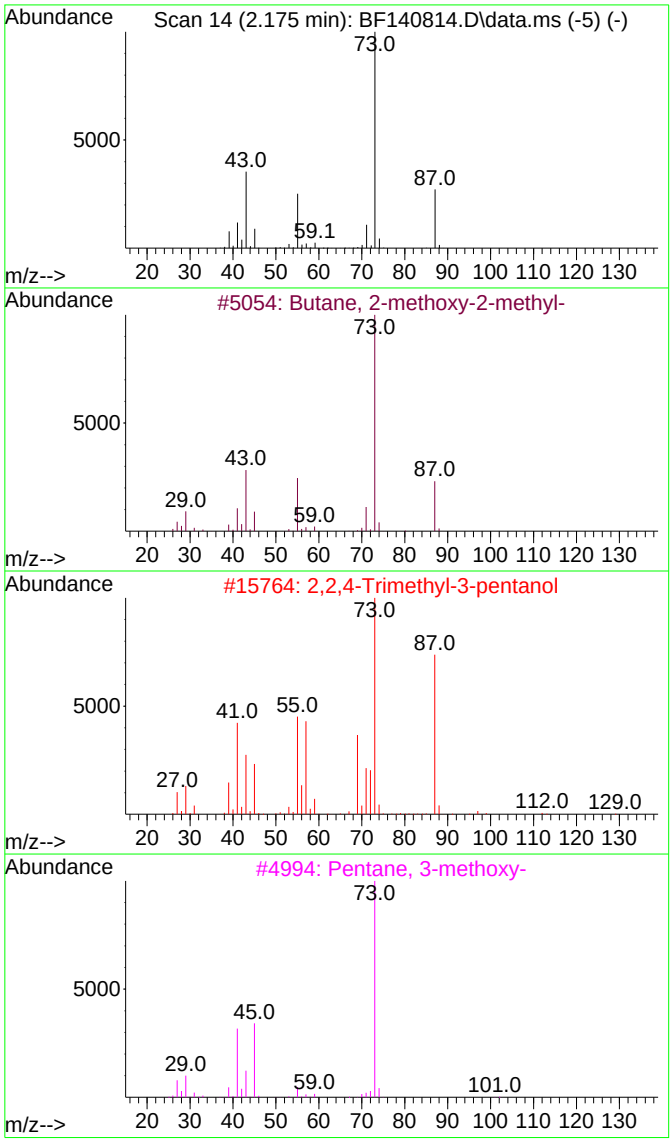
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

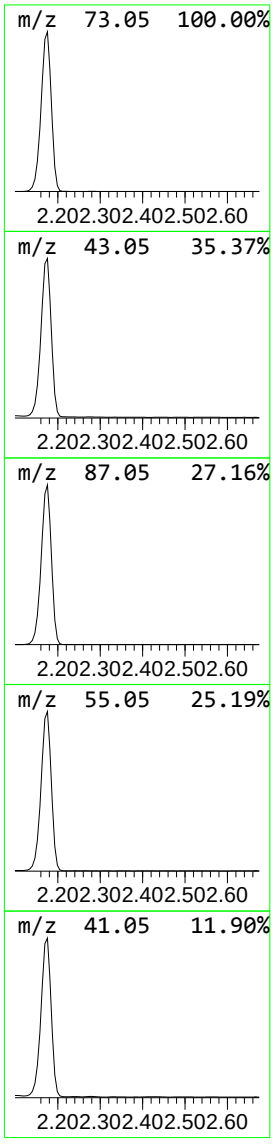
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	119.75 ng	2684650	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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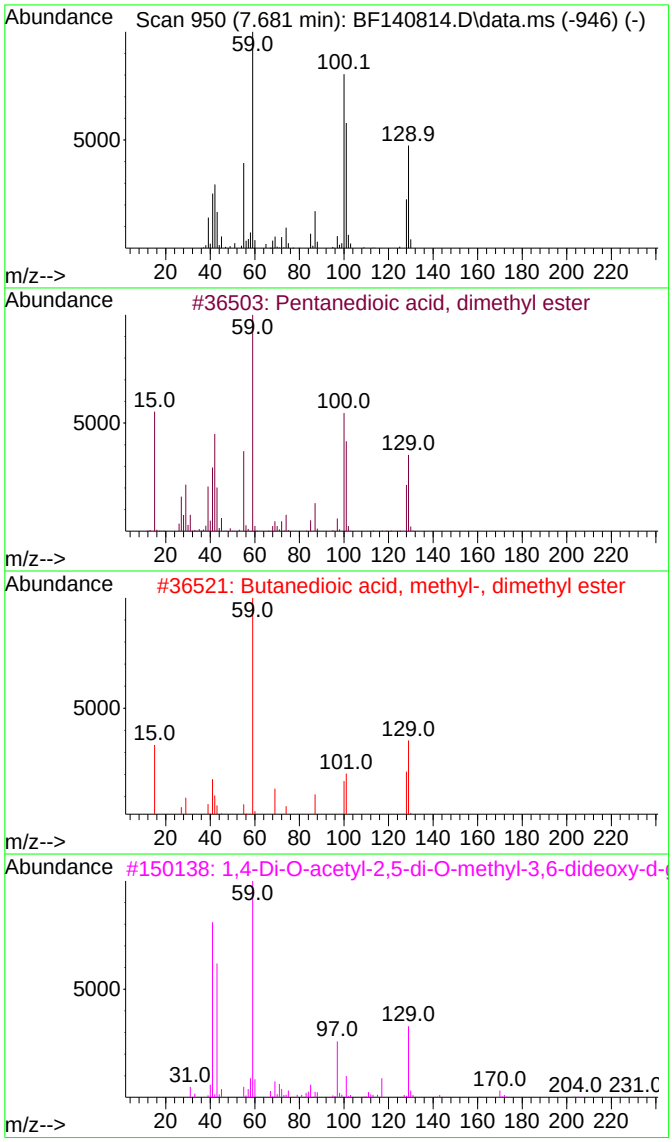
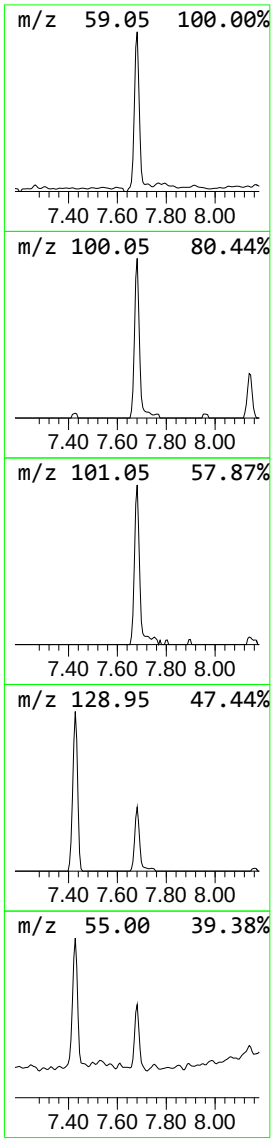
****
Peak Number 2 Pentanedioic acid, dimethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.681	2.38 ng	69318	Naphthalene-d8	8.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	64
2	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	47
3	1,4-Di-O-acetyl-2,5-di-O-methyl-...	262	C12H22O6	1000101-82-1	35
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
5	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	25





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Instrument :
BNA_F
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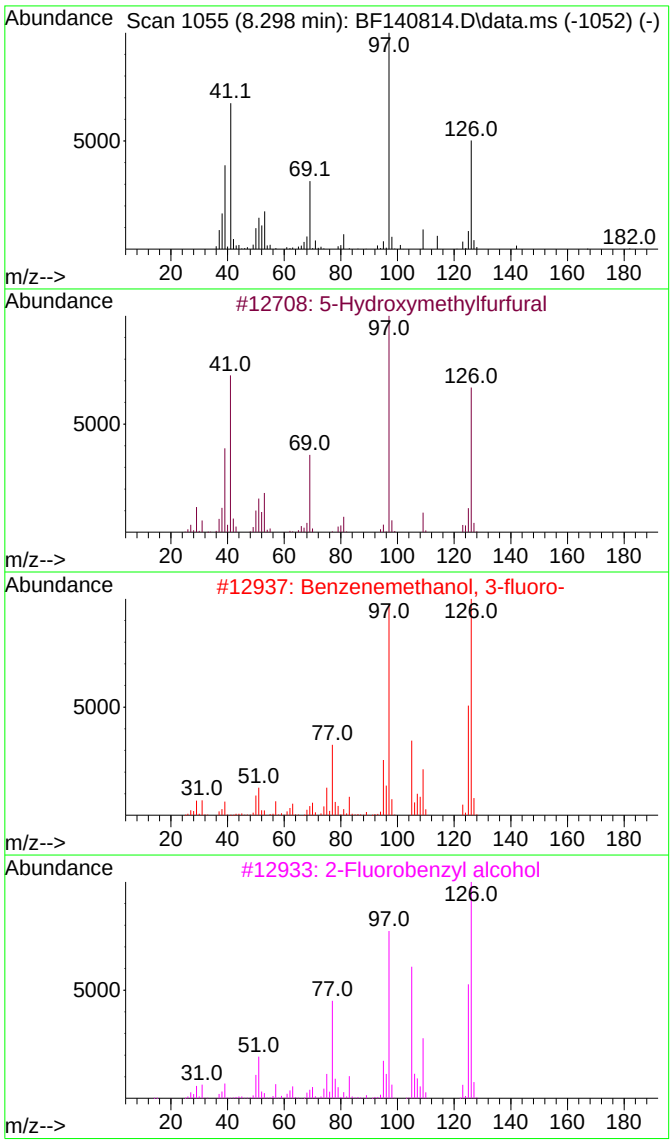
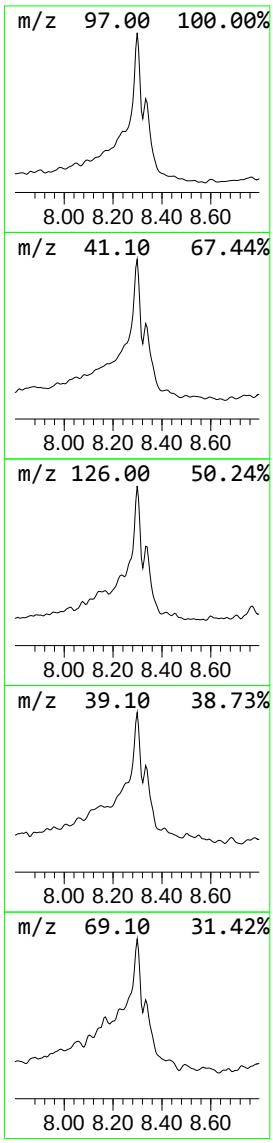
Peak Number 3 5-Hydroxymethylfurfural Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.298	2.59 ng	75662	Naphthalene-d8	8.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hydroxymethylfurfural	126	C6H6O3	000067-47-0	96
2	Benzenemethanol, 3-fluoro-	126	C7H7FO	000456-47-3	50
3	2-Fluorobenzyl alcohol	126	C7H7FO	000446-51-5	50
4	2-Fluoropyridine	97	C5H4FN	000372-48-5	27
5	1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	27





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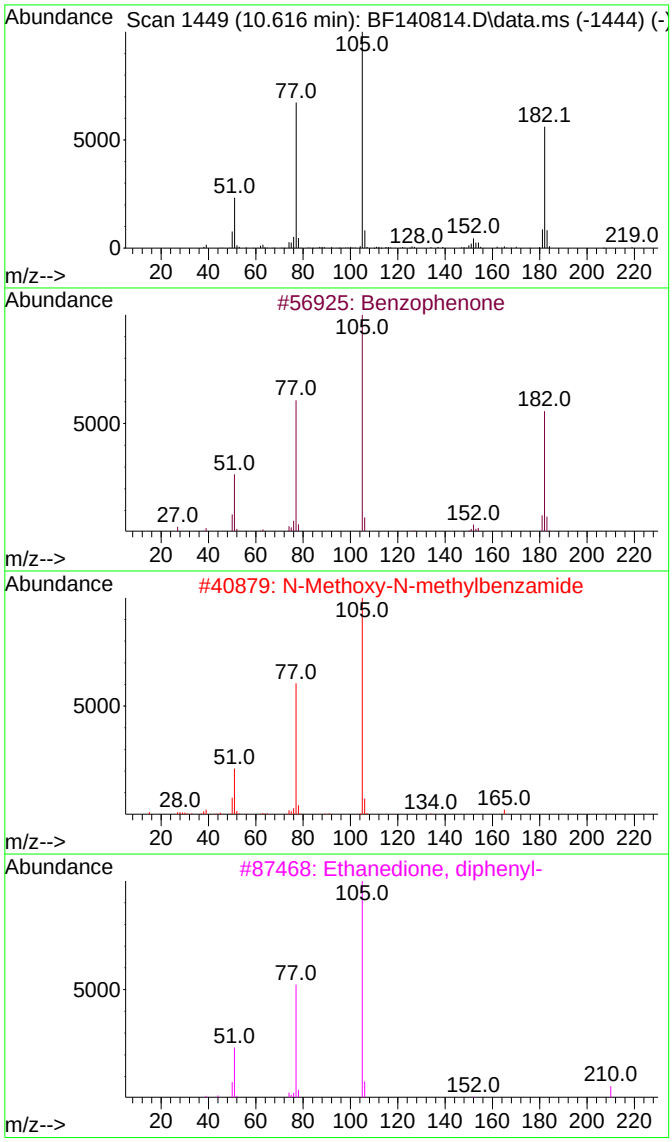
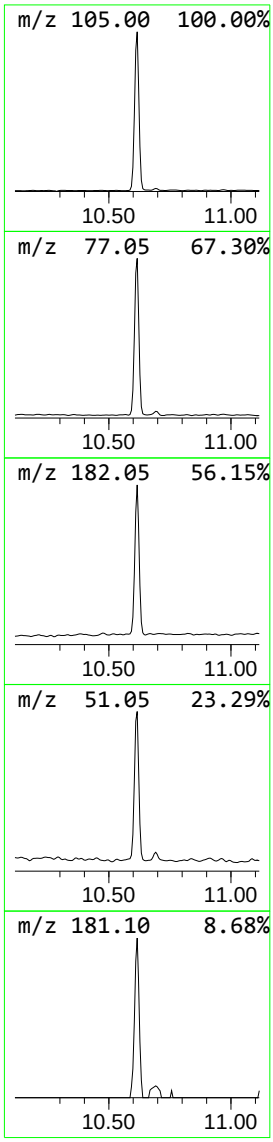
Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	2.16 ng	171556	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
3	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	47
4	N-[2,2-Dichloro-1-(toluene-4-sul...	371	C16H15Cl2NO3S	136800-77-6	47
5	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47





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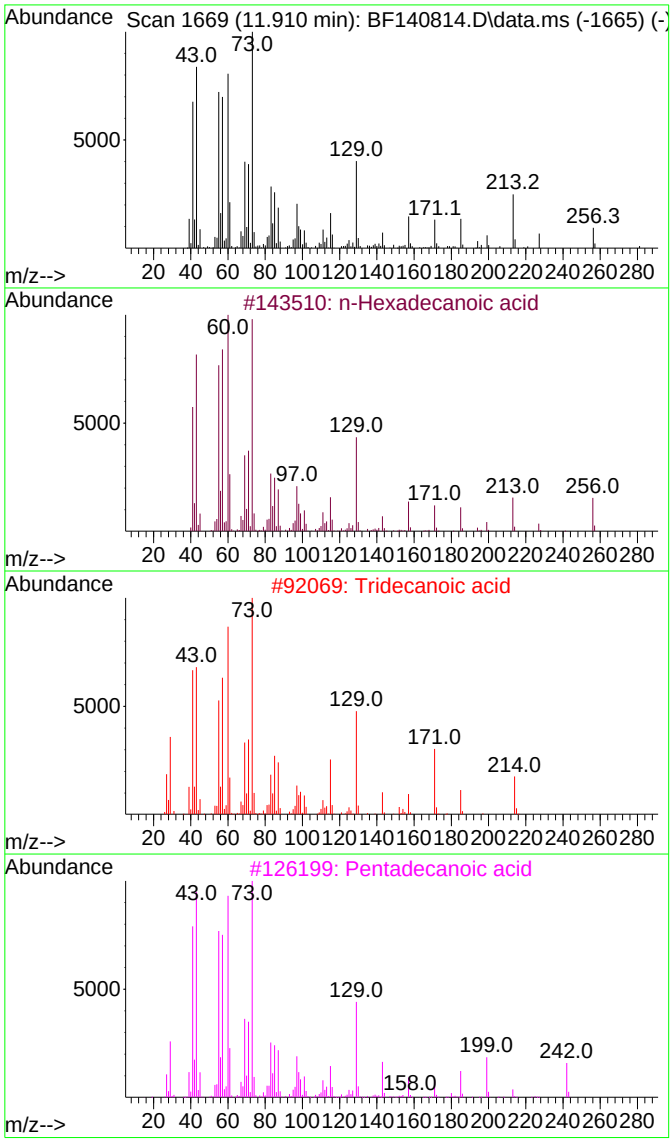
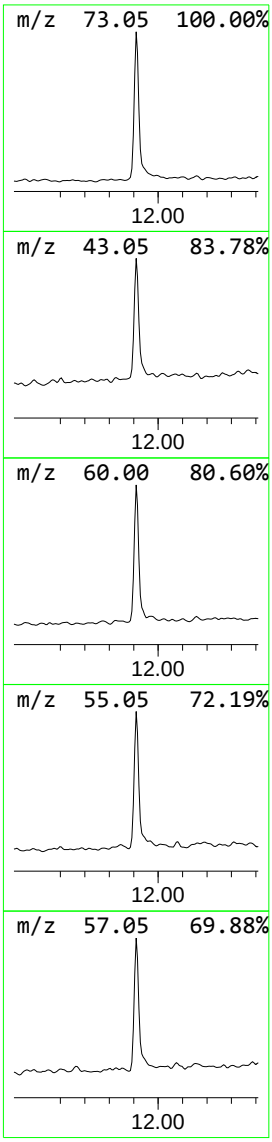
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	10.21 ng	278511	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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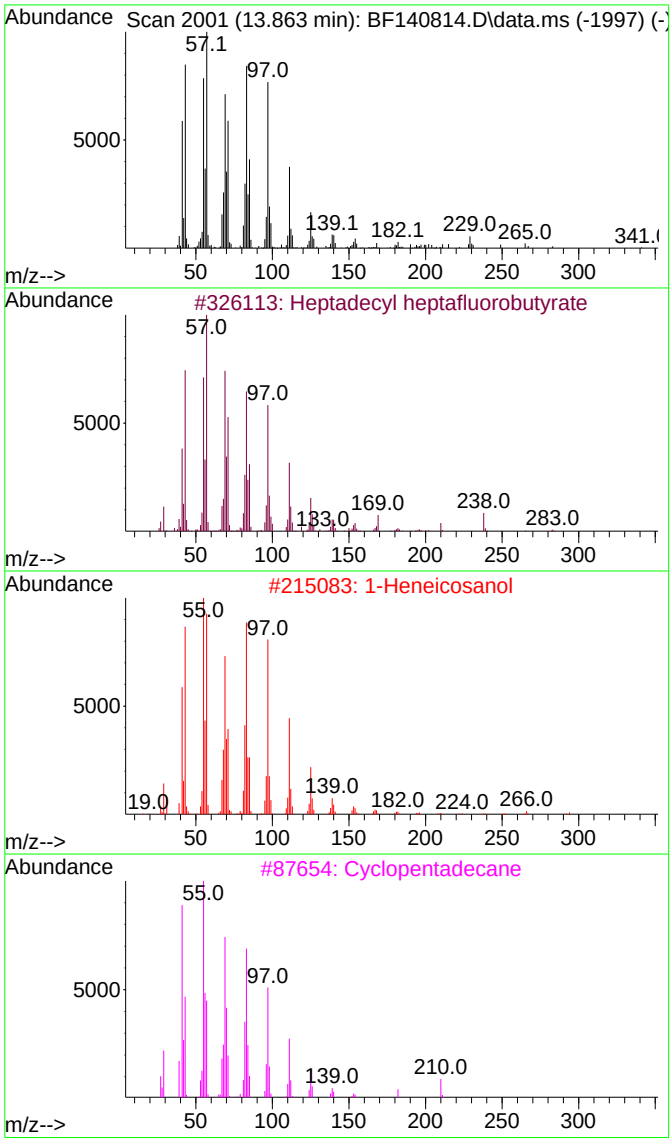
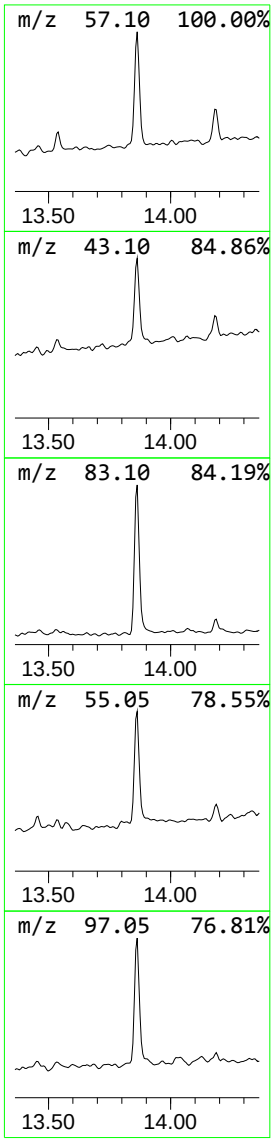
****
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	8.92 ng	179038	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Cyclopentadecane	210	C15H30	000295-48-7	92
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5	1-Tricosene	322	C23H46	018835-32-0	87





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...	2.175	119.8	ng	2684650	1	6.863	448376	20.0
Pentanedioic ac...	7.681	2.4	ng	69318	2	8.139	583419	20.0
5-Hydroxymethyl...	8.298	2.6	ng	75662	2	8.139	583419	20.0
Benzophenone	10.616	2.2	ng	171556	3	9.898	1585820	20.0
n-Hexadecanoic ...	11.910	10.2	ng	278511	4	11.392	545702	20.0
Heptadecyl hept...	13.863	8.9	ng	179038	5	14.045	401425	20.0