LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125652.D
Acq On : 25 Sep 2021 12:52
Operator : JU/CG
Sample : M3908-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-05-(23-25)

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-BF092421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125652.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	20	rBV	1059359	1321932	32.72%	4.889%
2	5.504	576	581	584	rBV	3151015	3024604	74.86%	11.186%
3	6.504	746	751	754	rBV	3123469	3081884	76.28%	11.398%
4	6.886	812	816	819	rBV	1086663	830385	20.55%	3.071%
5	7.445	906	911	914	rBV	2296930	1979586	49.00%	7.321%
6	8.063	1013	1016	1026	rBV	256817	228372	5.65%	0.845%
7	8.169	1030	1034	1037	rVV	1365662	1153609	28.55%	4.266%
8	9.245	1212	1217	1220	rBV	4486900	4040244	100.00%	14.942%
9	9.922	1328	1332	1335	rBV	1658551	1322984	32.75%	4.893%
10	10.704	1461	1465	1469	rBV	2652633	2415152	59.78%	8.932%
11	11.404	1580	1584	1588	rBV	1595232	1291318	31.96%	4.776%
12	11.927	1668	1673	1678	rBV	183525	178943	4.43%	0.662%
13	12.710	1803	1806	1815	rBV	56640	70904	1.75%	0.262%
14	12.992	1849	1854	1857	rBV	4148899	3688165	91.29%	13.640%
15	13.468	1931	1935	1942	rBV	69241	64004	1.58%	0.237%
16	13.839	1979	1998	2000	rBV6	52332	184450	4.57%	0.682%
17	13.892	2003	2007	2015	rVB4	89252	172649	4.27%	0.638%
18	14.039	2028	2032	2036	rVB	1190315	965913	23.91%	3.572%
19	14.457	2089	2103	2107	rBV7	22994	86347	2.14%	0.319%
20	15.004	2185	2196	2207	rVB7	25509	96671	2.39%	0.358%
21	15.515	2278	2283	2287	rBV	650938	797884	19.75%	2.951%
22	16.004	2360	2366	2371	rBV2	22141	43790	1.08%	0.162%

Sum of corrected areas: 27039790

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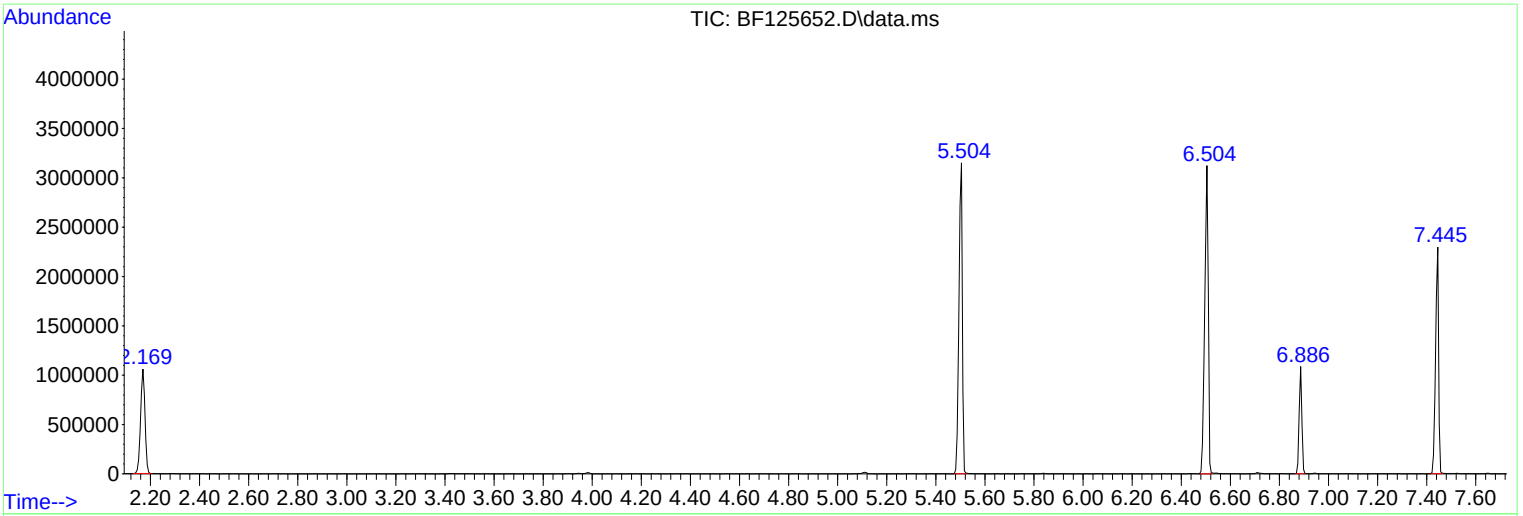
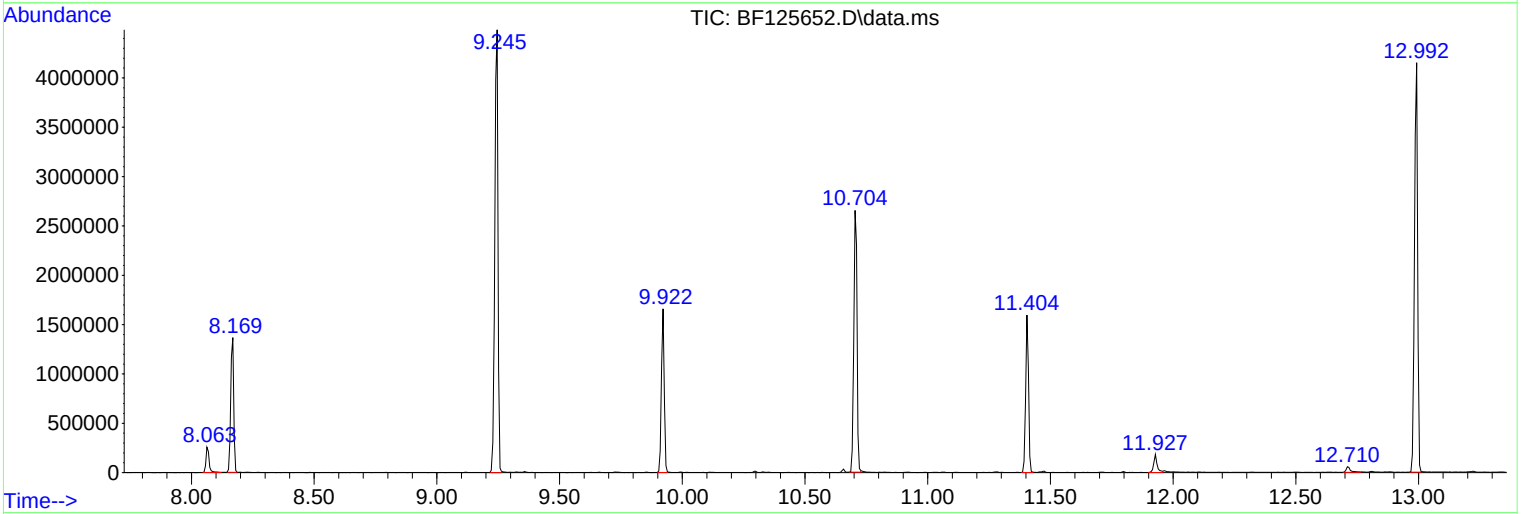
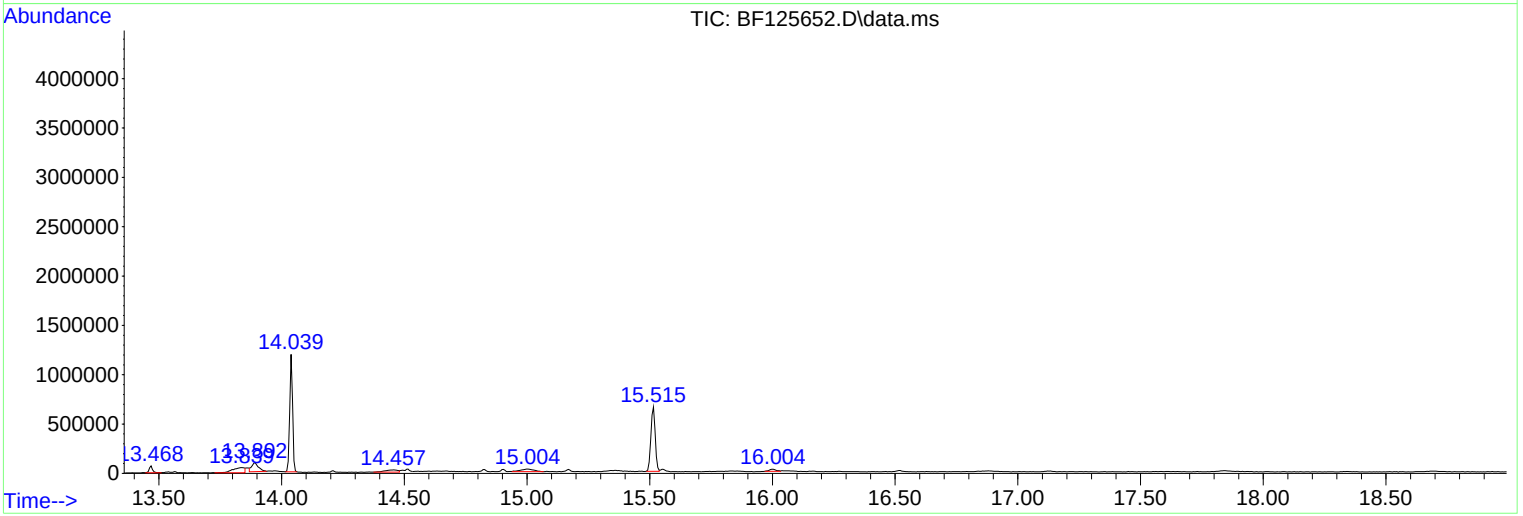
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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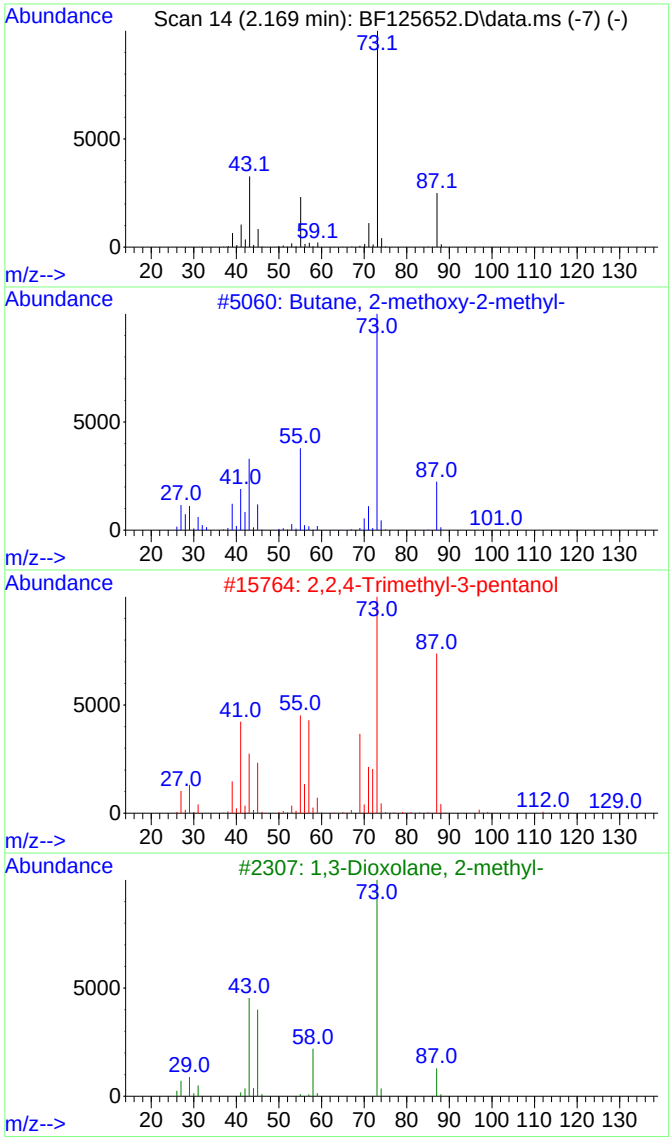
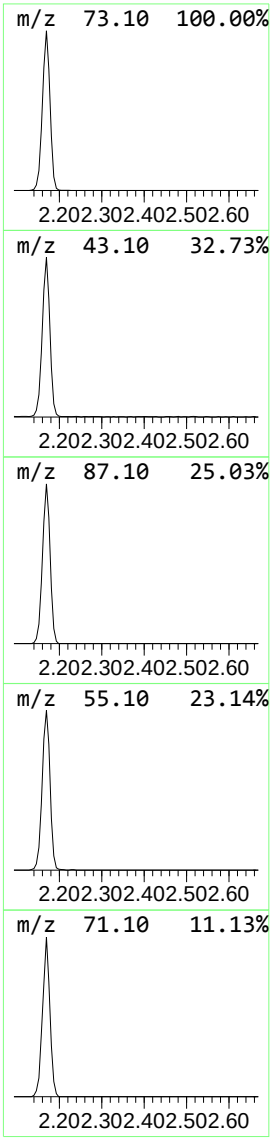
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	31.84 ng	1321930	1,4-Dichlorobenzene-d4	6.886

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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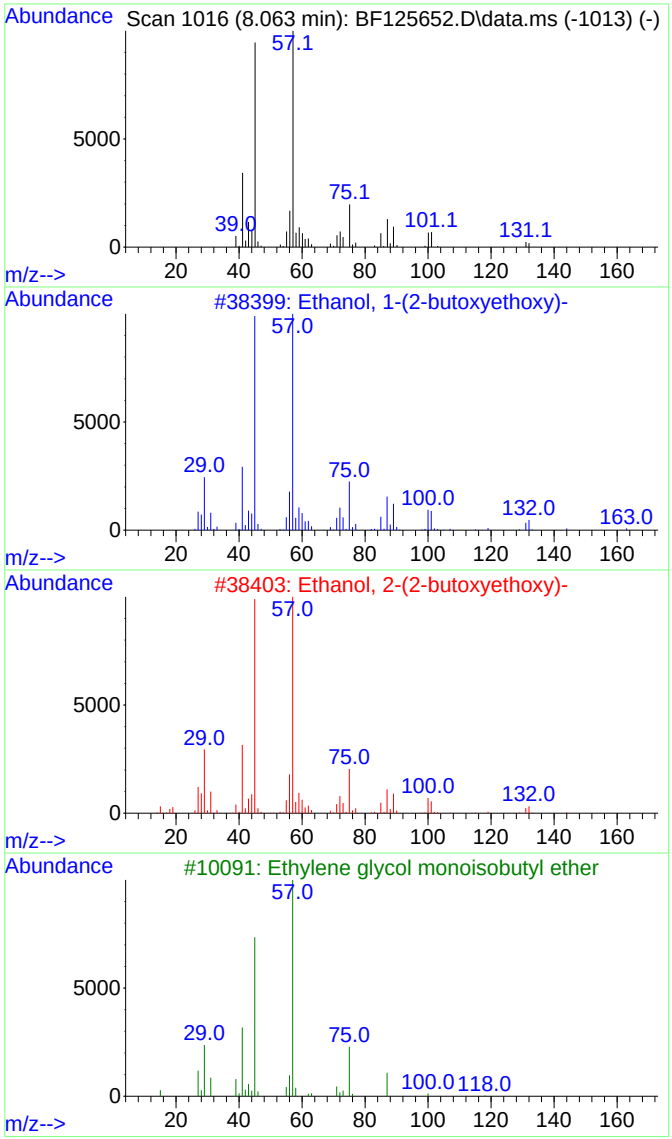
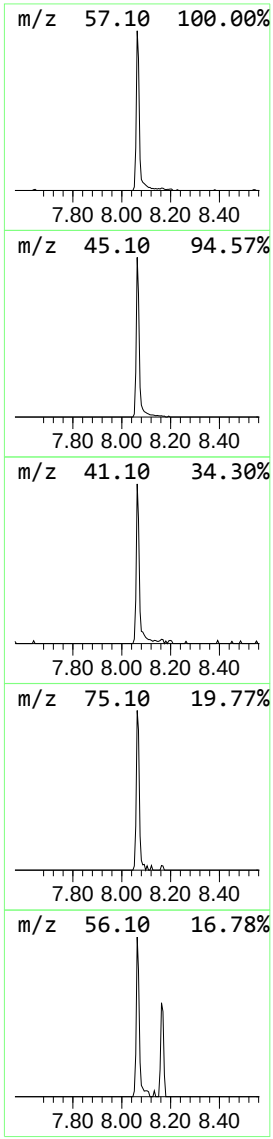
****
Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.063	3.96 ng	228372	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50





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Sample : M3908-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
SUP-UST-05-(23-25)

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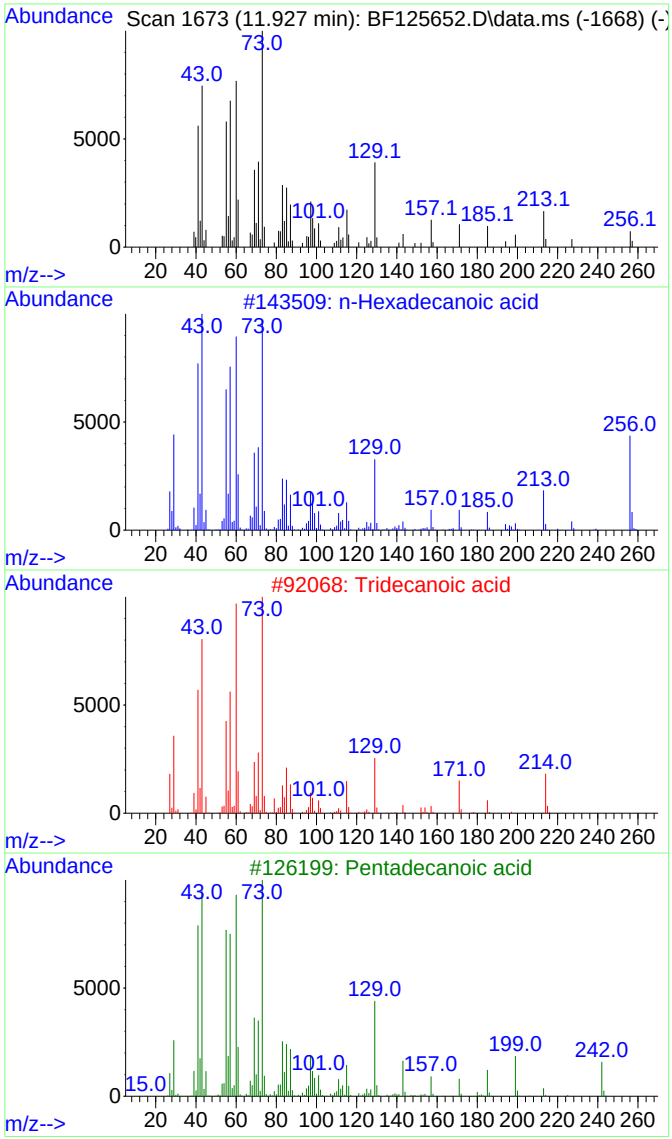
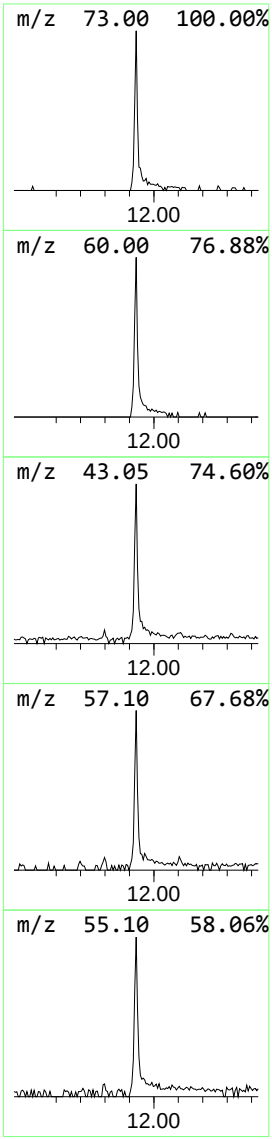
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	2.77 ng	178943	Phenanthrene-d10	11.404

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	90
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20





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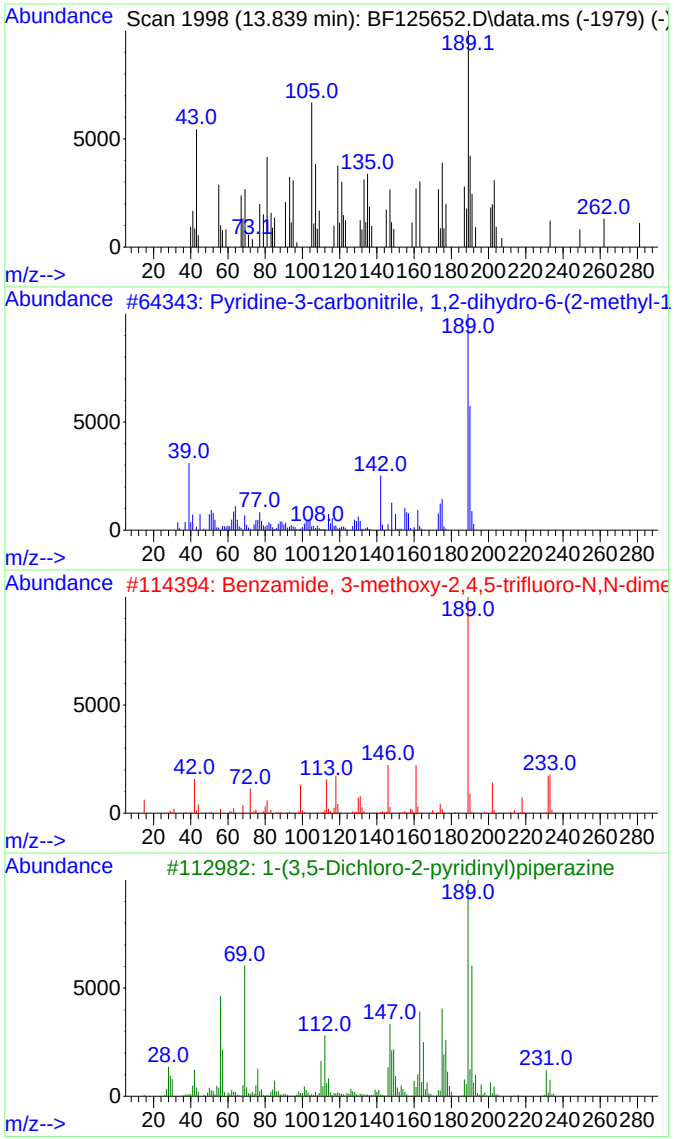
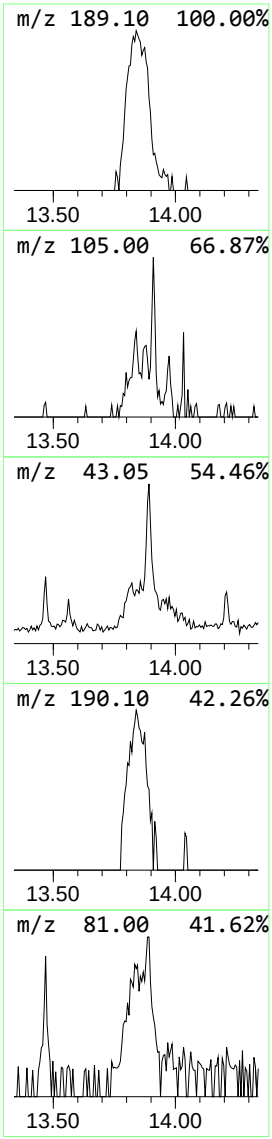
Peak Number 4 unknown13.839 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	3.82 ng	184450	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-3-carbonitrile, 1,2-dih...	190	C10H10N2S	202270-50-6	35
2	Benzamide, 3-methoxy-2,4,5-trifl...	233	C10H10F3NO2	1000437-07-4	27
3	1-(3,5-Dichloro-2-pyridinyl)pipe...	231	C9H11Cl2N3	087394-60-3	25
4	2-((2S,4aR)-4a,8-Dimethyl-1,2,3,...	222	C15H26O	117066-77-0	25
5	Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	25





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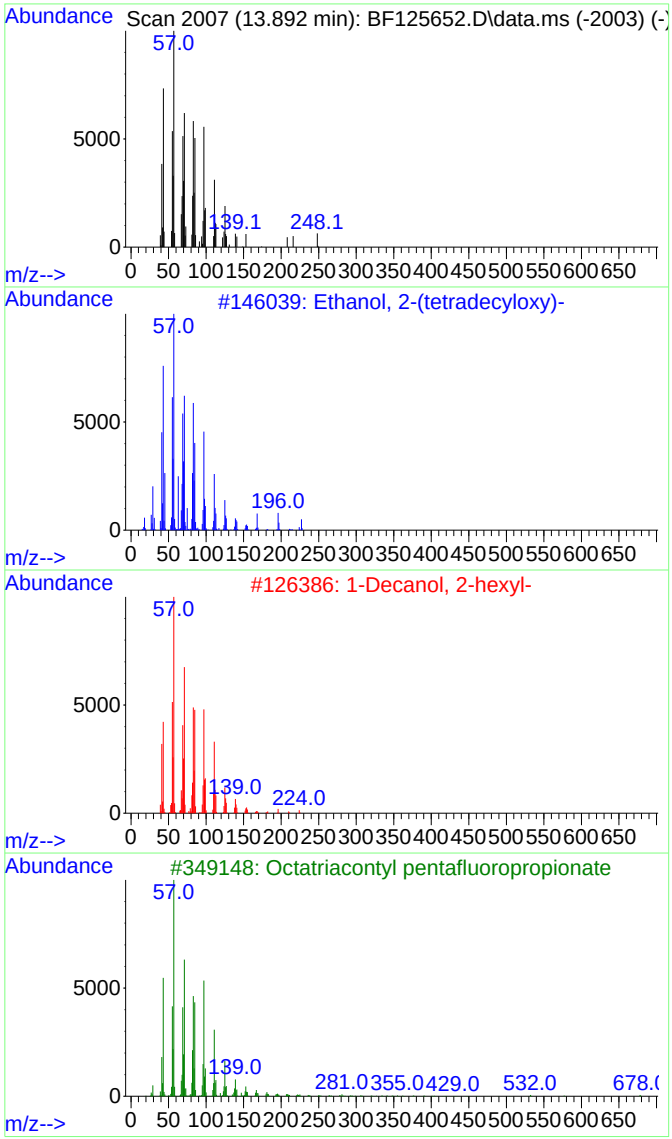
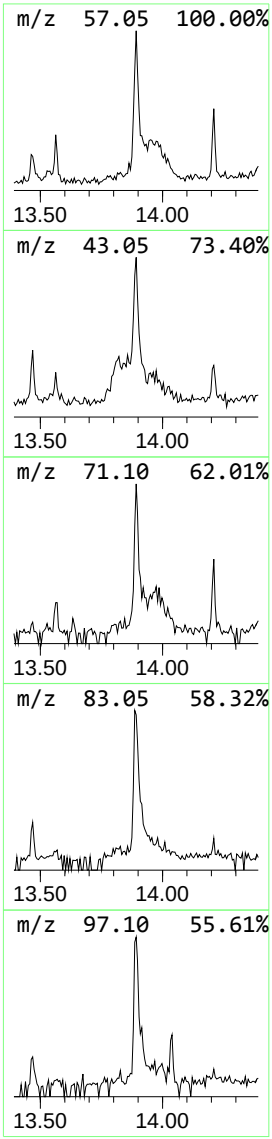
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.57 ng	172649	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
3	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	87
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	83





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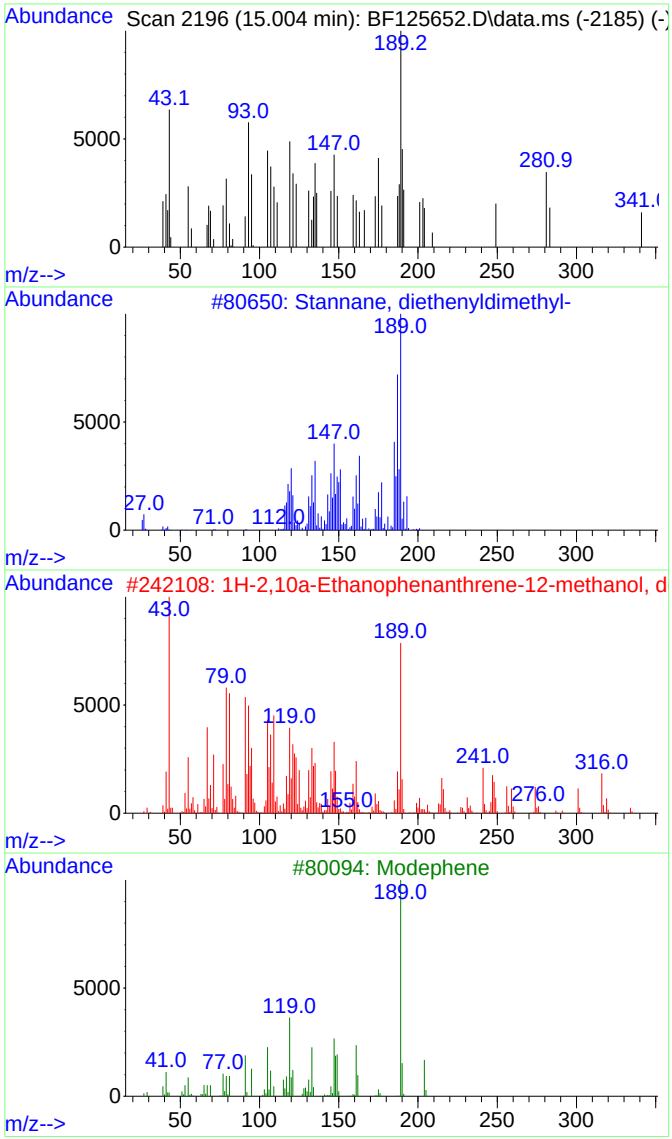
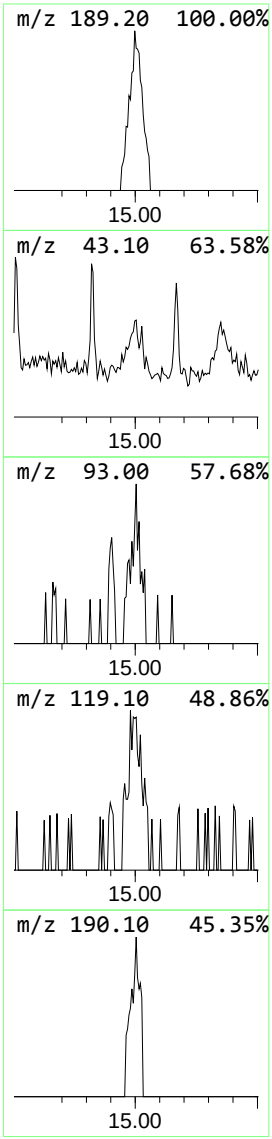
Peak Number 6 unknown15.004 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	2.42 ng	96671	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stannane, diethenyldimethyl-	204	C6H12Sn	020204-11-9	38
2	1H-2,10a-Ethanophenanthrene-12-m...	334	C21H34O3	1000504-06-9	38
3	Modephene	204	C15H24	068269-87-4	27
4	Benzeneacetic acid, .alpha.-meth...	234	C10H9F3O3	020445-31-2	27
5	5-((1S,2R,4aR)-5-(Acetoxymethyl)...	364	C22H36O4	1000495-83-8	25





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.169	31.8	ng	1321930	1	6.886	830385	20.0
Ethanol, 1-(2-b...	8.063	4.0	ng	228372	2	8.169	1153610	20.0
n-Hexadecanoic ...	11.927	2.8	ng	178943	4	11.404	1291320	20.0
unknown13.839	13.839	3.8	ng	184450	5	14.039	965913	20.0
Ethanol, 2-(tet...	13.892	3.6	ng	172649	5	14.039	965913	20.0
unknown15.004	15.004	2.4	ng	96671	6	15.515	797884	20.0