LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092321\
Data File : BF125602.D
Acq On : 23 Sep 2021 20:45
Operator : JU/CG
Sample : M3889-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-04-(6-8)

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-BF092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125602.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	10	19	26	rVB	1520211	1945503	30.56%	4.397%
2	5.516	577	583	586	rBV	4769741	4797377	75.36%	10.843%
3	6.516	747	753	756	rBV	4479441	4815053	75.64%	10.882%
4	6.892	814	817	821	rVB	1449739	1150528	18.07%	2.600%
5	7.451	907	912	915	rBV	3114966	3191497	50.13%	7.213%
6	8.075	1014	1018	1021	rBV	843487	672926	10.57%	1.521%
7	8.175	1031	1035	1038	rBV	1966355	1612734	25.33%	3.645%
8	9.251	1213	1218	1221	rBV	6583746	6116917	96.09%	13.825%
9	9.928	1329	1333	1337	rBV	2021197	1857936	29.18%	4.199%
10	10.716	1463	1467	1471	rBV	3846977	3875280	60.87%	8.758%
11	11.416	1582	1586	1589	rBV	2306947	1889307	29.68%	4.270%
12	11.939	1670	1675	1680	rBV	633982	595258	9.35%	1.345%
13	12.645	1790	1795	1802	rBV3	46078	73307	1.15%	0.166%
14	12.727	1805	1809	1819	rVV	249301	255726	4.02%	0.578%
15	13.004	1851	1856	1859	rBV	6283645	6366081	100.00%	14.388%
16	13.898	2005	2008	2020	rBV	503372	604742	9.50%	1.367%
17	14.057	2030	2035	2038	rBV	1789024	1700175	26.71%	3.843%
18	14.221	2060	2063	2070	rBV	74994	76087	1.20%	0.172%
19	14.527	2112	2115	2122	rBV2	121716	161072	2.53%	0.364%
20	14.839	2165	2168	2172	rBV	57723	63798	1.00%	0.144%
21	14.921	2178	2182	2190	rVB	716872	692177	10.87%	1.564%
22	15.186	2223	2227	2231	rBV	74094	84331	1.32%	0.191%
23	15.533	2280	2286	2291	rBV	1227860	1554597	24.42%	3.514%
24	16.080	2374	2379	2387	rBV	44437	93530	1.47%	0.211%

Sum of corrected areas: 44245939

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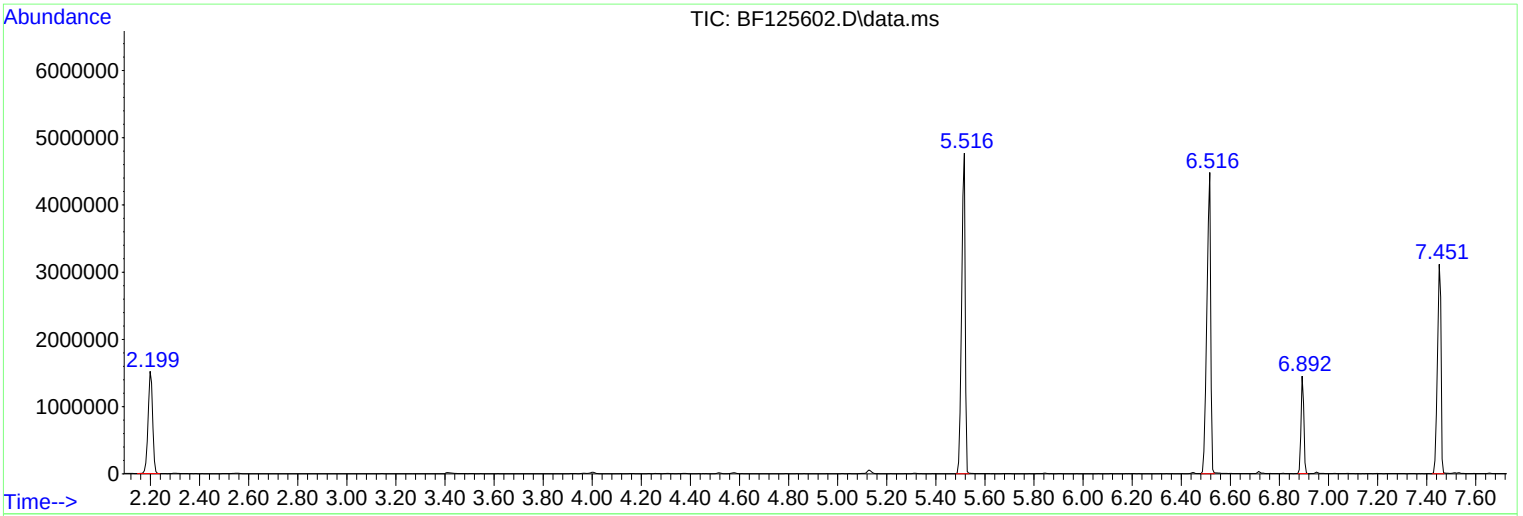
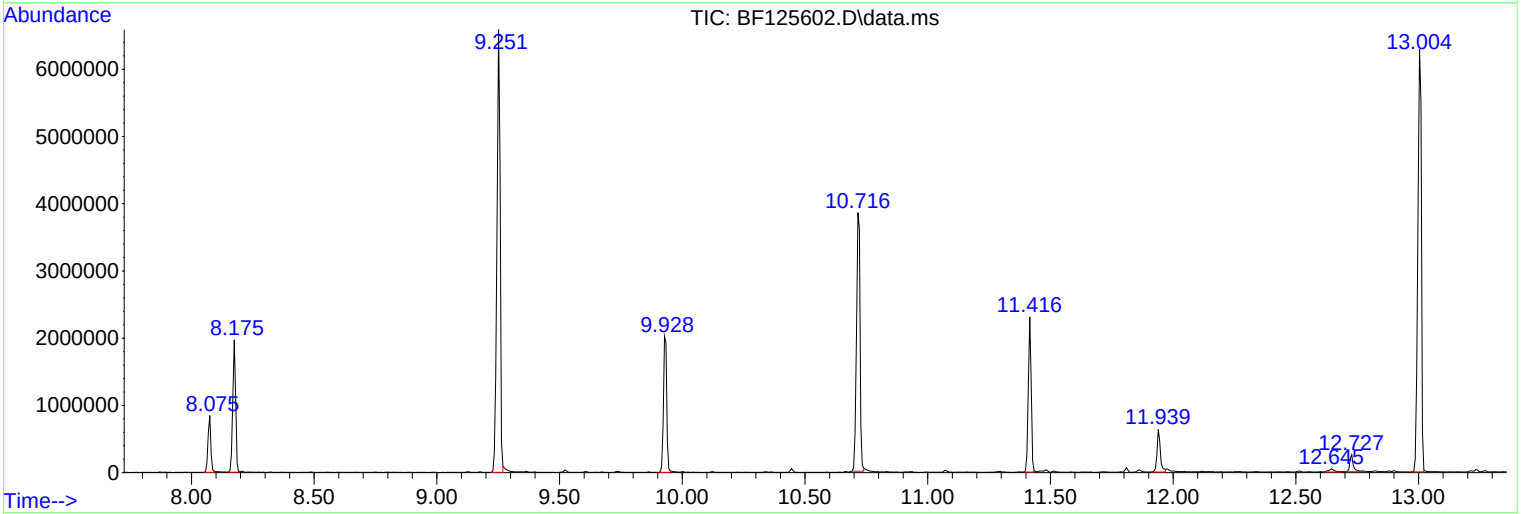
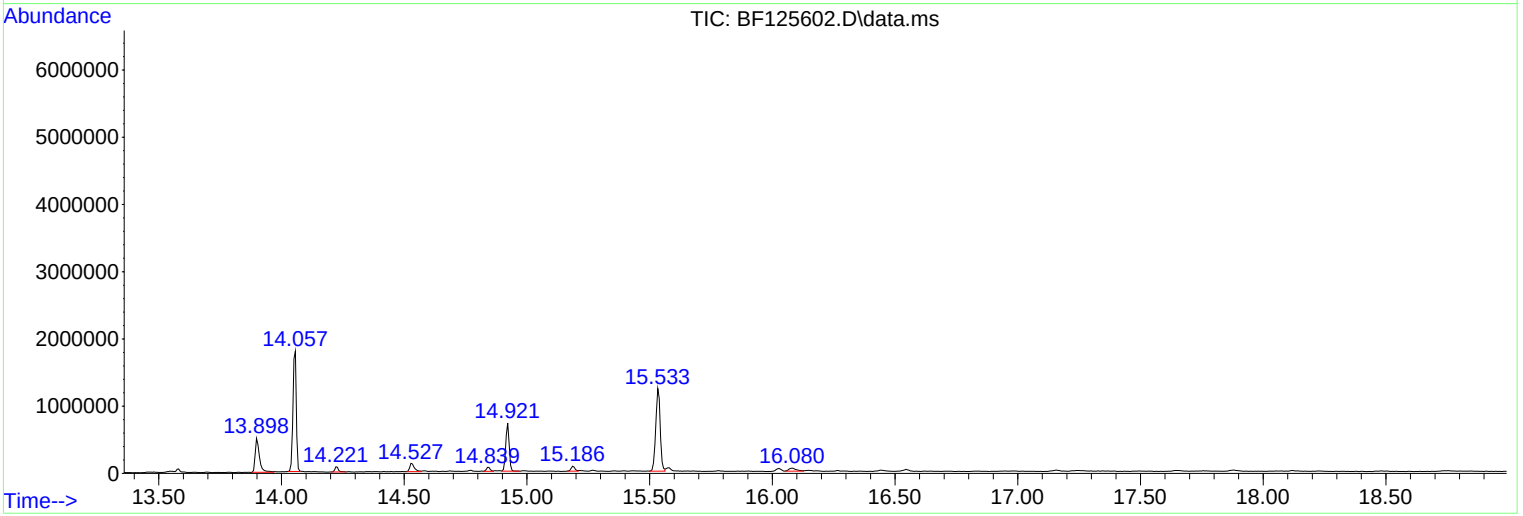
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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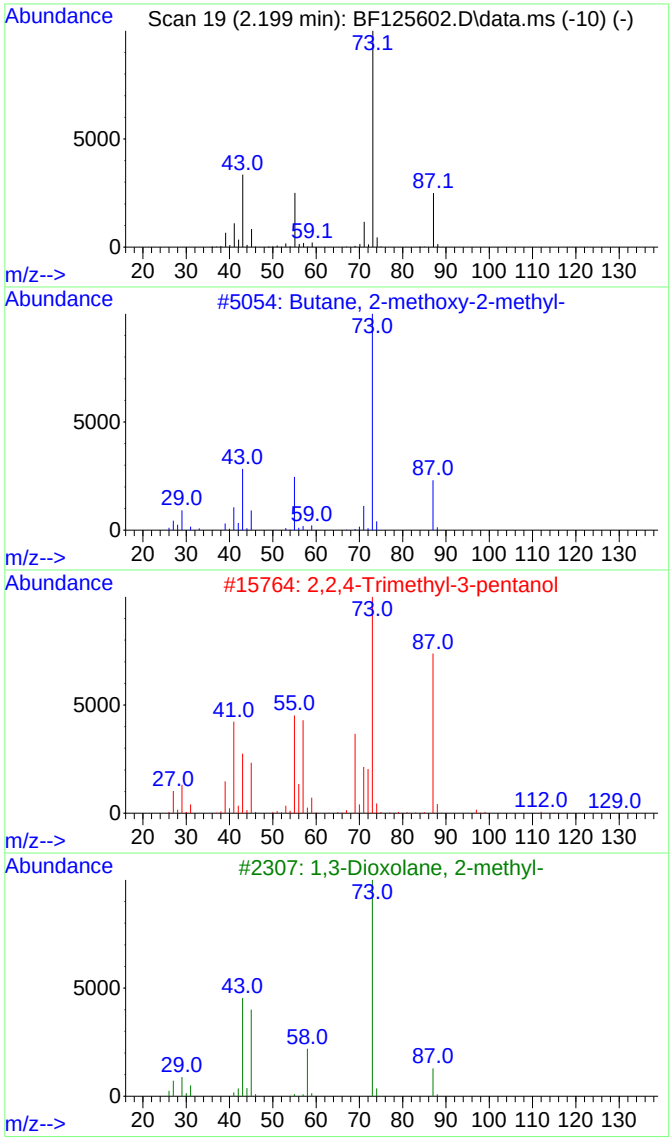
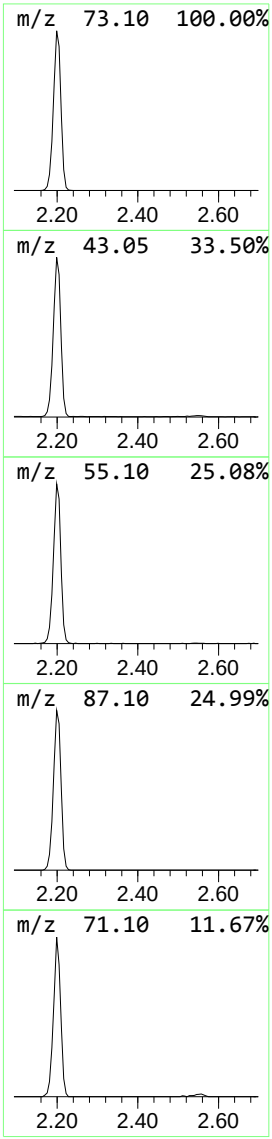
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	33.82 ng	1945500	1,4-Dichlorobenzene-d4	6.892

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	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	9





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-04-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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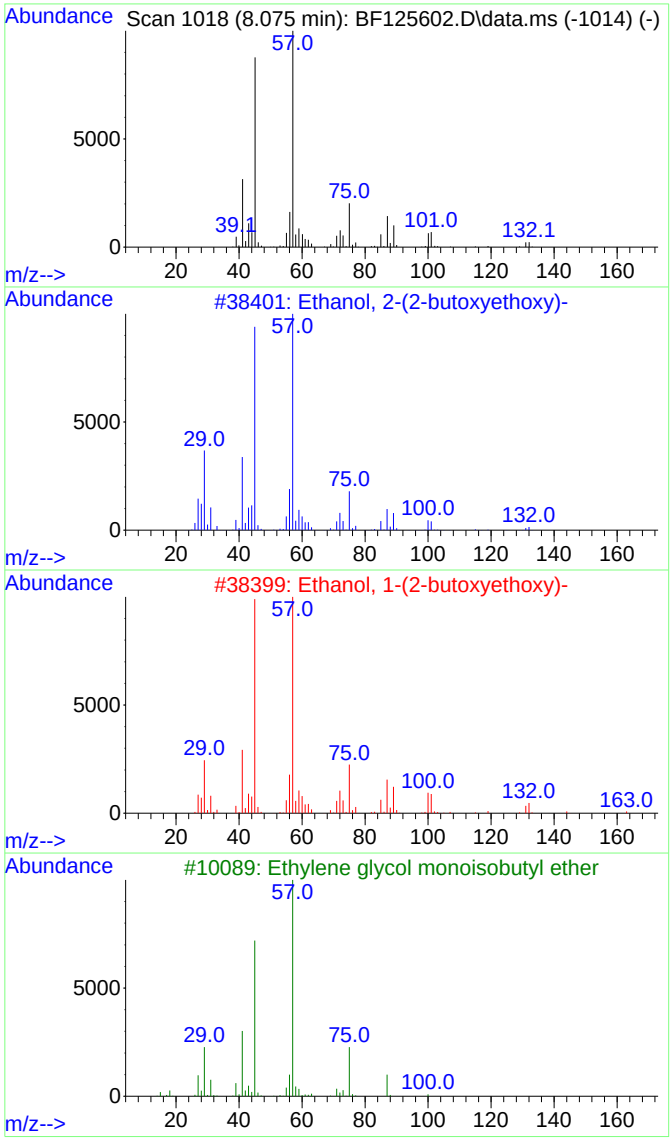
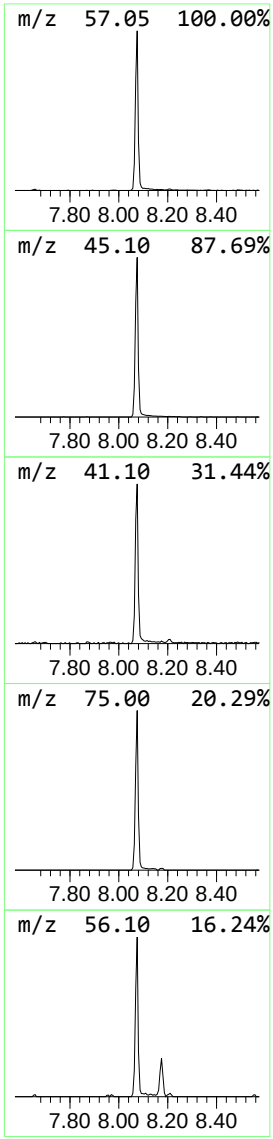
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	8.35 ng	672926	Naphthalene-d8	8.175

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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50





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Instrument : BNA_F
ClientSampleId : SUP-UST-04-(6-8)

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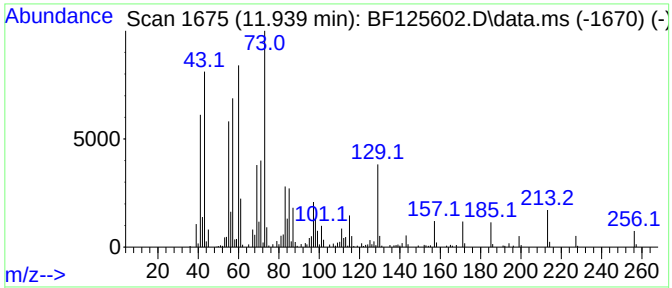
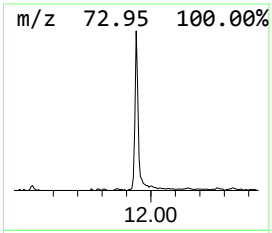
****

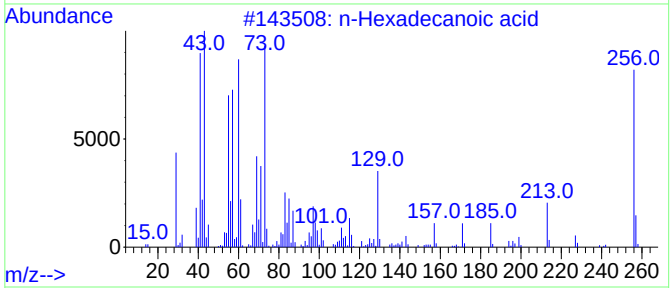
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

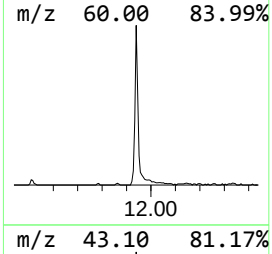
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	6.30 ng	595258	Phenanthrene-d10	11.416

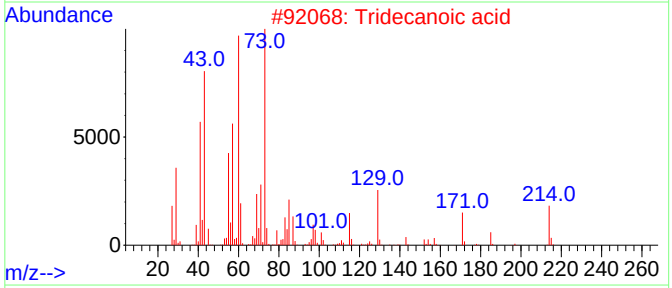
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62

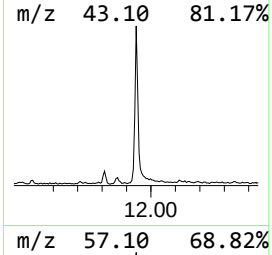


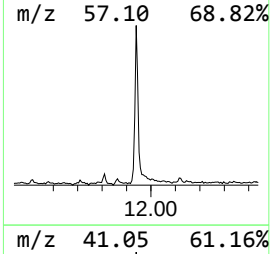


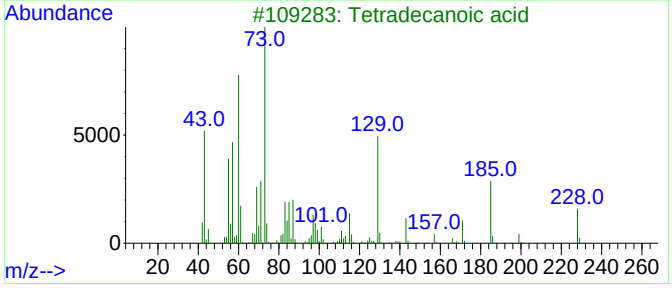


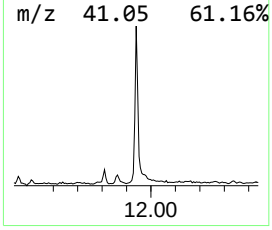












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SUP-UST-04-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

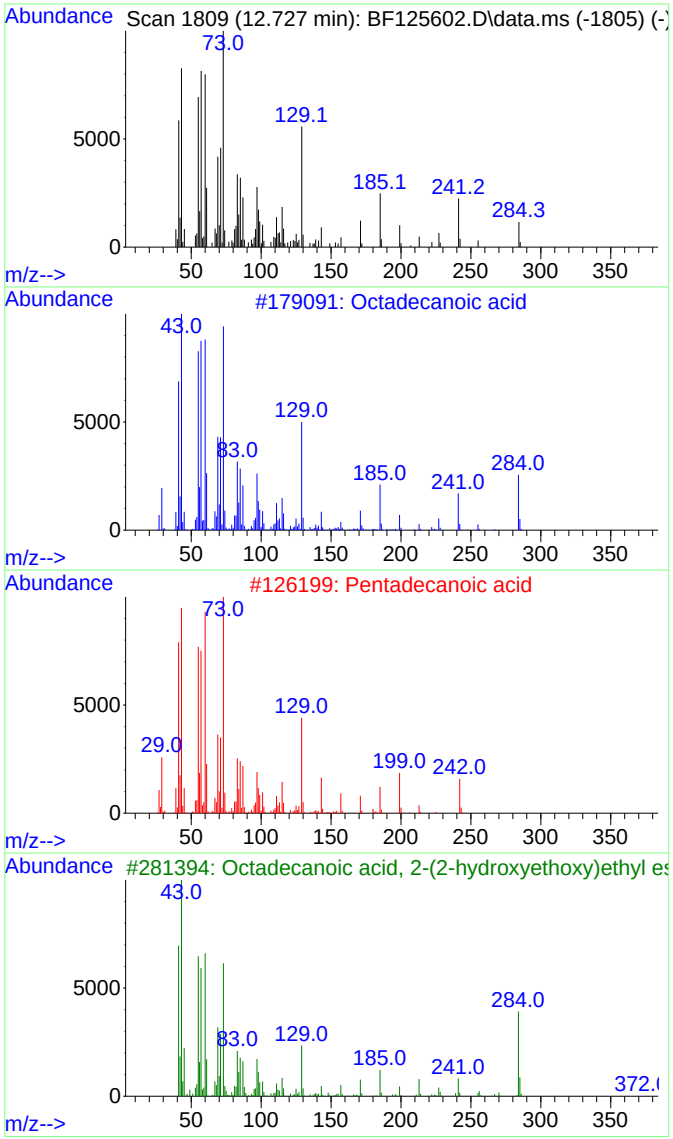
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

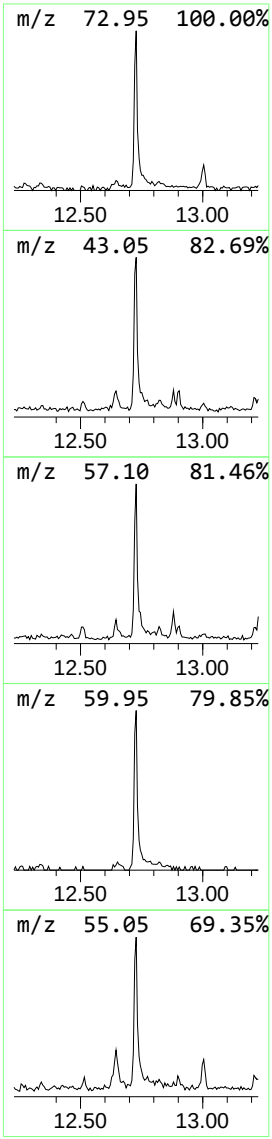
****

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	2.71 ng	255726	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80





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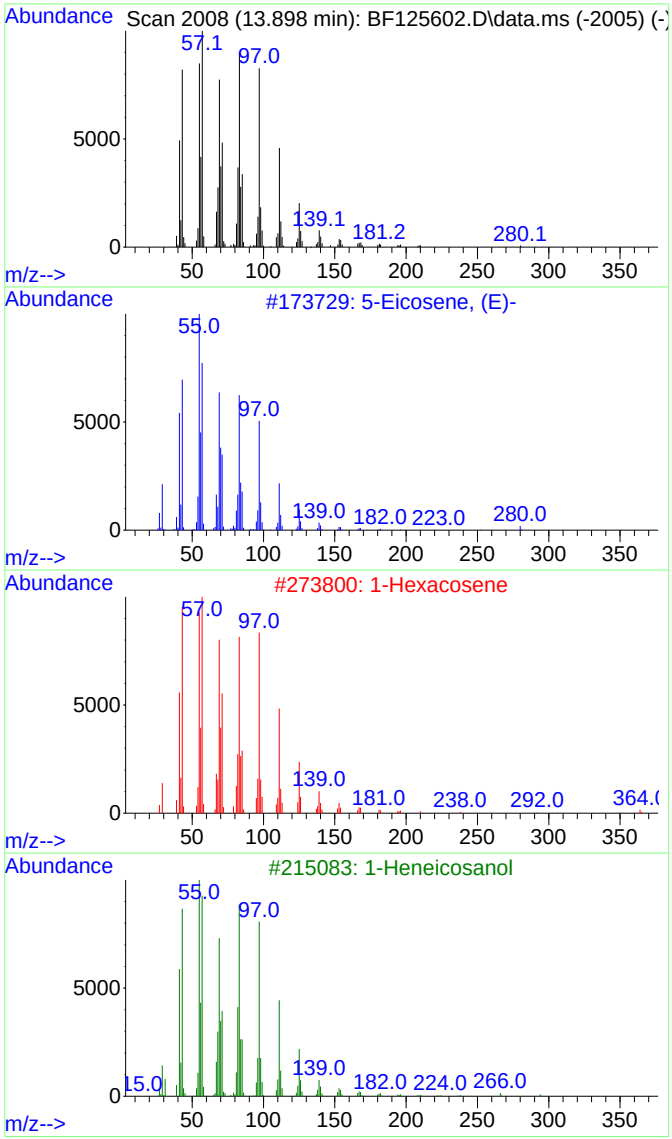
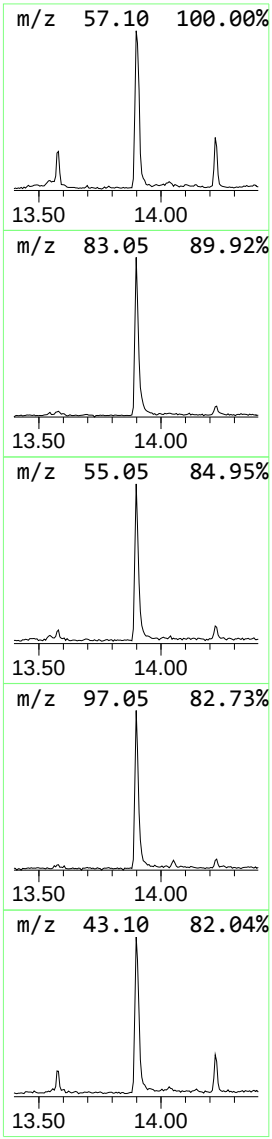
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	7.11 ng	604742	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	1-Hexacosene	364	C26H52	018835-33-1	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





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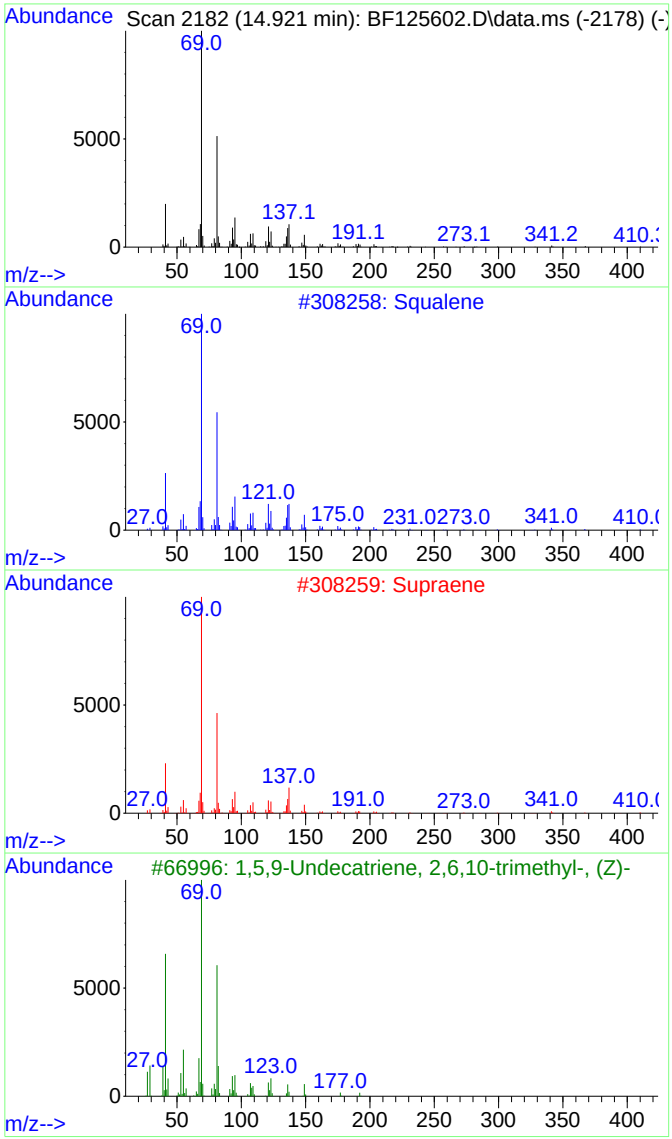
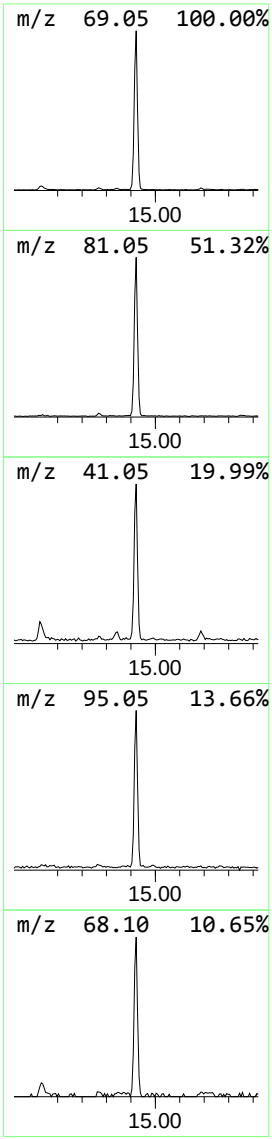
Peak Number 6 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	8.90 ng	692177	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	95
2	Supraene	410	C30H50	007683-64-9	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50





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...	2.199	33.8	ng	1945500	1	6.892	1150530	20.0
Ethanol, 2-(2-b...	8.075	8.3	ng	672926	2	8.175	1612730	20.0
n-Hexadecanoic ...	11.939	6.3	ng	595258	4	11.416	1889310	20.0
Octadecanoic acid	12.727	2.7	ng	255726	4	11.416	1889310	20.0
5-Eicosene, (E)-	13.898	7.1	ng	604742	5	14.057	1700180	20.0
Squalene	14.921	8.9	ng	692177	6	15.533	1554600	20.0