LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114445.D
Acq On : 21 May 2019 2:43
Operator : JU/SJ
Sample : K2943-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-2

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-BF051019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.463	570	574	596	rBV	4949929	5068586	91.03%	10.152%
2	6.475	741	746	764	rBV	5018000	5368350	96.41%	10.752%
3	6.604	764	768	776	rVB	5516312	5056144	90.81%	10.127%
4	6.828	802	806	815	rBV	1356824	1132044	20.33%	2.267%
5	6.987	829	833	836	rBV	4271905	3938544	70.73%	7.889%
6	7.392	897	902	919	rBV	3297148	3388528	60.86%	6.787%
7	8.110	1020	1024	1040	rBV	1478979	1421351	25.53%	2.847%
8	9.186	1202	1207	1210	rBV	5780872	5466009	98.17%	10.948%
9	9.580	1270	1274	1285	rBV	751132	756119	13.58%	1.514%
10	9.863	1319	1322	1335	rVB	1711718	1578593	28.35%	3.162%
11	10.657	1453	1457	1466	rBV	3660448	3543577	63.64%	7.098%
12	11.351	1571	1575	1582	rBV	1901978	1704599	30.61%	3.414%
13	11.874	1661	1664	1676	rBV	407389	474551	8.52%	0.950%
14	12.580	1779	1784	1790	rBV6	26216	57669	1.04%	0.116%
15	12.657	1794	1797	1806	rVV	75257	100953	1.81%	0.202%
16	12.933	1839	1844	1847	rBV	5647059	5568085	100.00%	11.153%
17	13.157	1877	1882	1893	rBV2	42796	78157	1.40%	0.157%
18	13.827	1992	1996	2013	rBV2	384815	897943	16.13%	1.799%
19	13.992	2020	2024	2032	rVB	1561346	1521925	27.33%	3.048%
20	14.439	2097	2100	2103	rBV2	106317	119773	2.15%	0.240%
21	14.474	2103	2106	2115	rVB6	47167	106842	1.92%	0.214%
22	14.745	2148	2152	2155	rBV	110529	108034	1.94%	0.216%
23	15.074	2204	2208	2213	rBV	207231	211380	3.80%	0.423%
24	15.457	2267	2273	2284	rBV	1122787	1492601	26.81%	2.990%
25	15.651	2302	2306	2310	rVB	44821	62716	1.13%	0.126%
26	15.874	2339	2344	2351	rBV	154296	227193	4.08%	0.455%
27	15.992	2353	2364	2371	rBV8	53174	187170	3.36%	0.375%
28	16.374	2424	2429	2432	rBV	37429	60630	1.09%	0.121%
29	16.945	2522	2526	2535	rVB3	32502	65742	1.18%	0.132%
30	17.045	2538	2543	2549	rBV9	45884	91326	1.64%	0.183%
31	17.121	2552	2556	2567	rVB9	27414	71498	1.28%	0.143%

Sum of corrected areas: 49926632

LSC Report - Integrated Chromatogram

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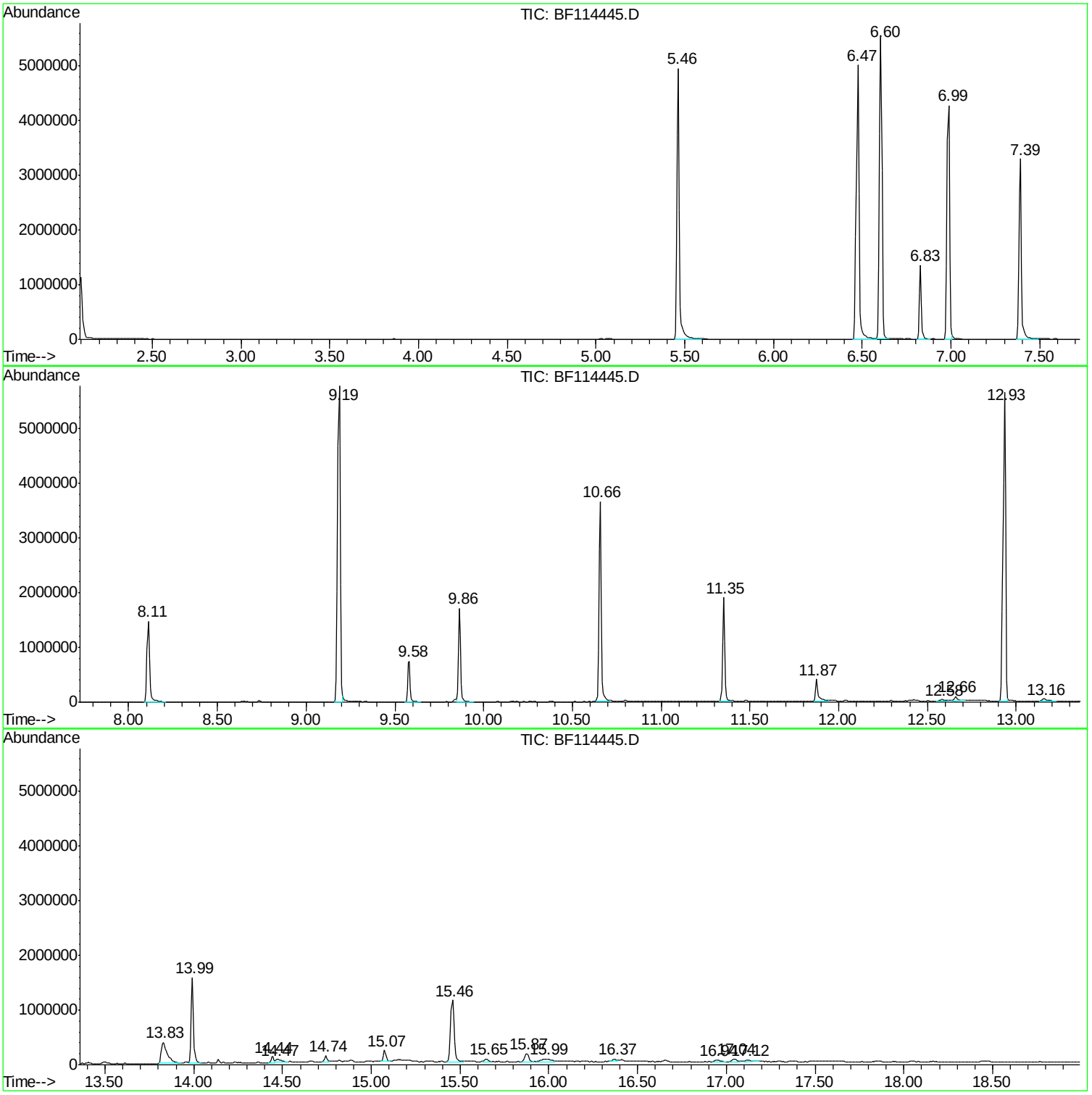
Sample : K2943-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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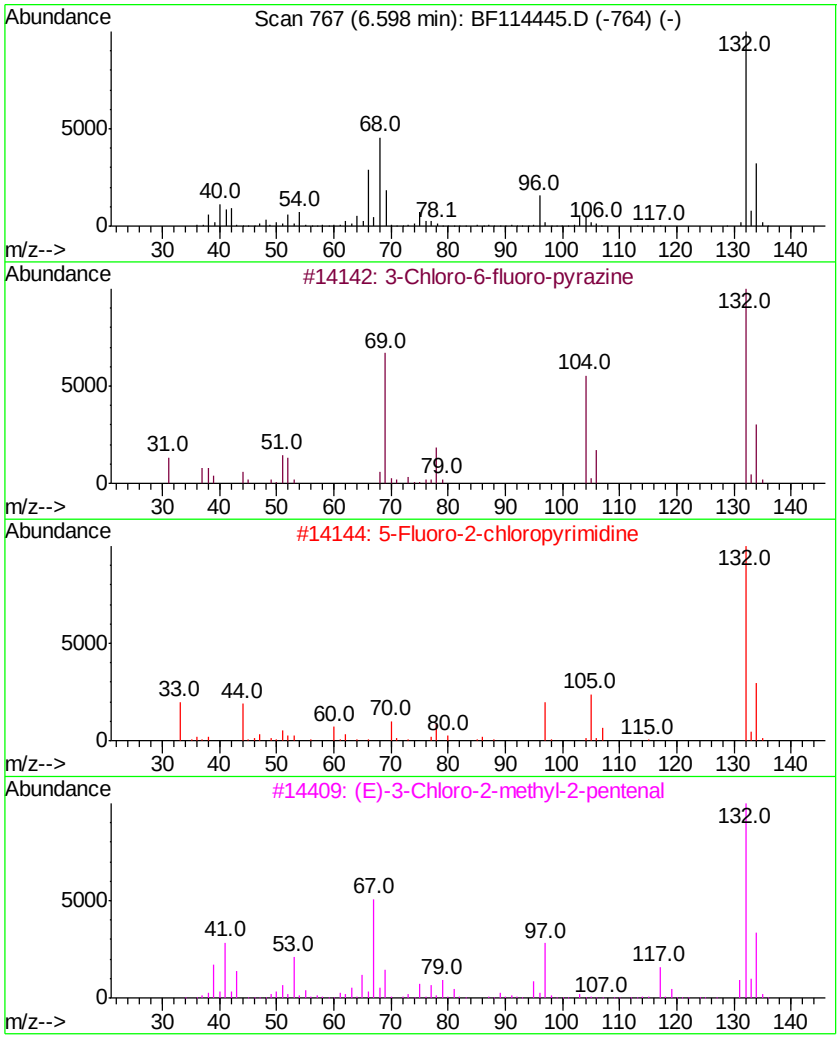
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

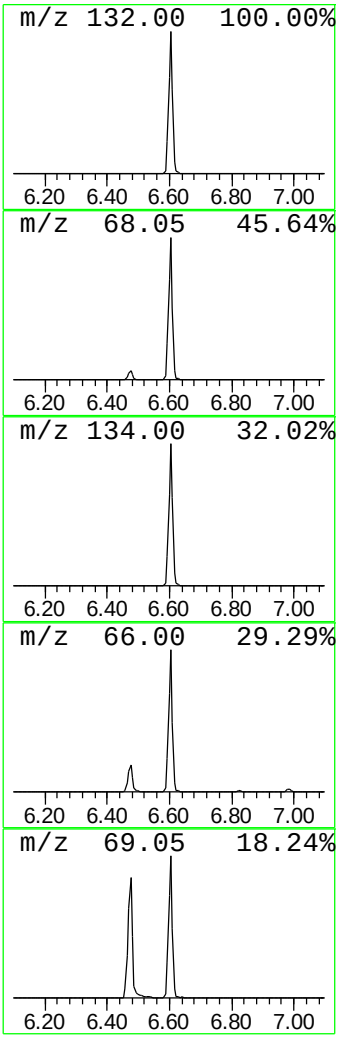
****

Peak Number 1 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	89.33 ng	5056140	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

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Data File : BF114445.D
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Misc :
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Instrument : BNA_F
ClientSampleId : BUS-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
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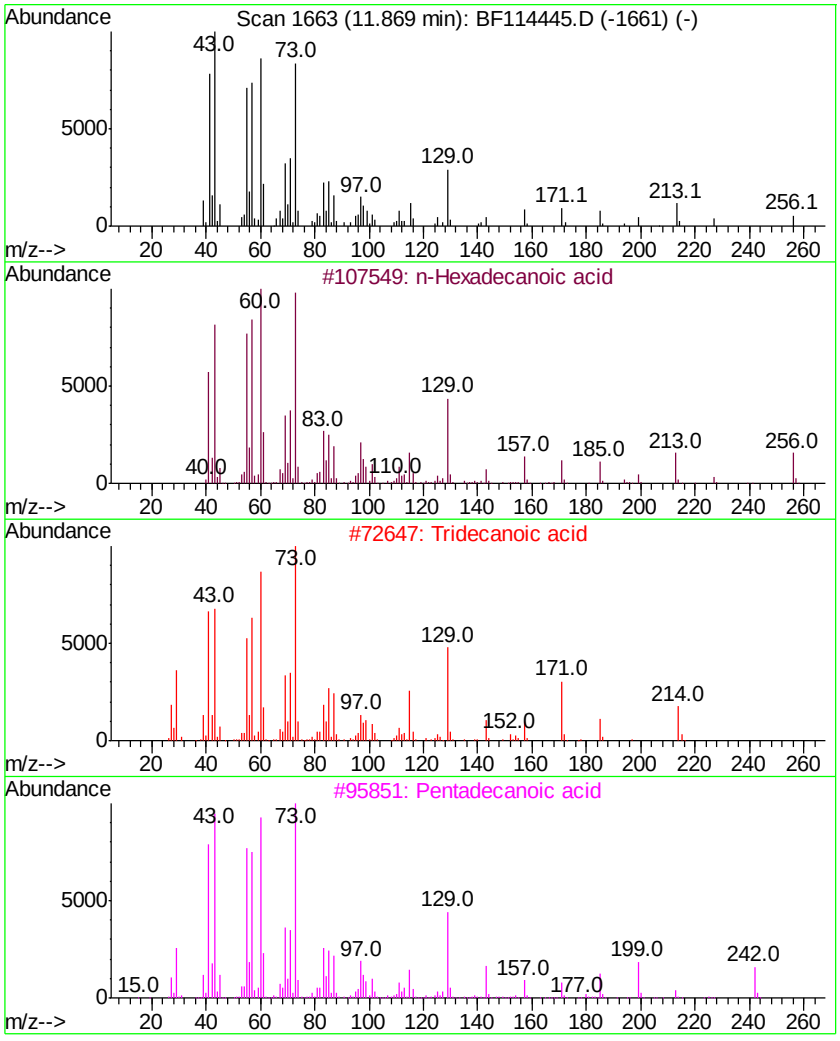
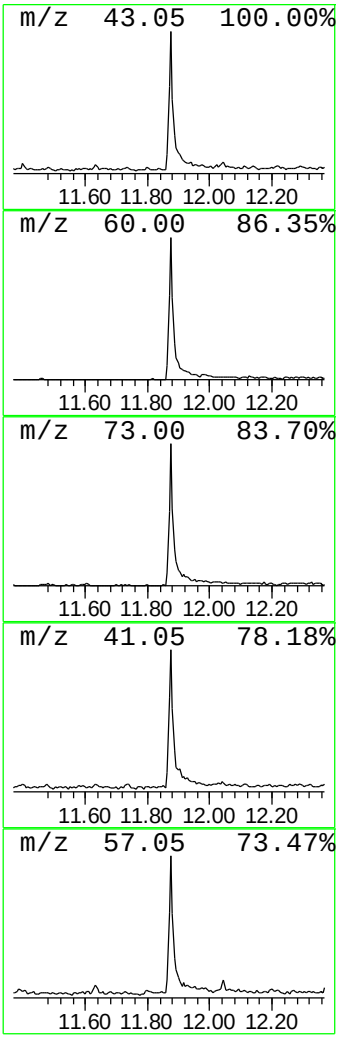
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	5.57 ng	474551	Phenanthrene-d10	11.35

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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Sample : K2943-13
Misc :
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Instrument : BNA_F
ClientSampleId : BUS-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
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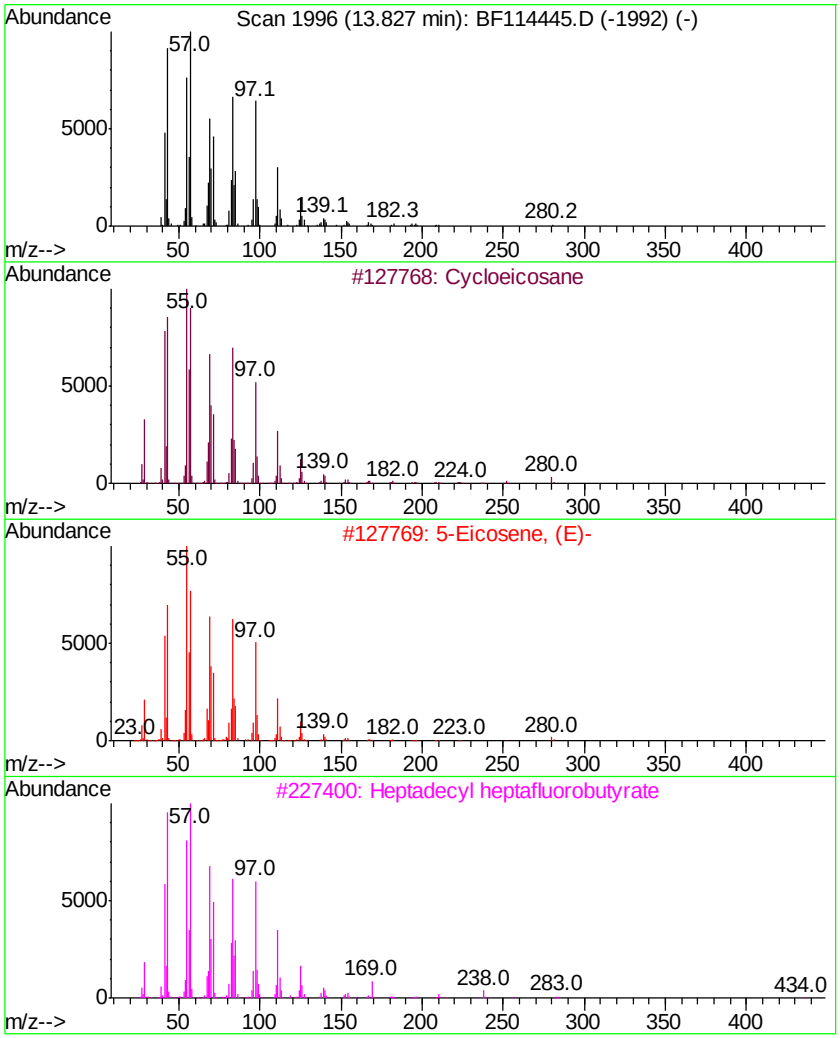
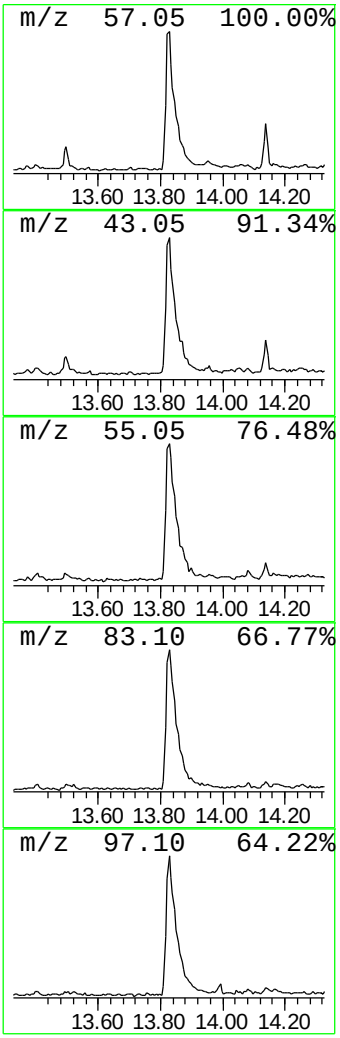
Peak Number 4 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	11.80 ng	897943	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	96
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : BUS-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
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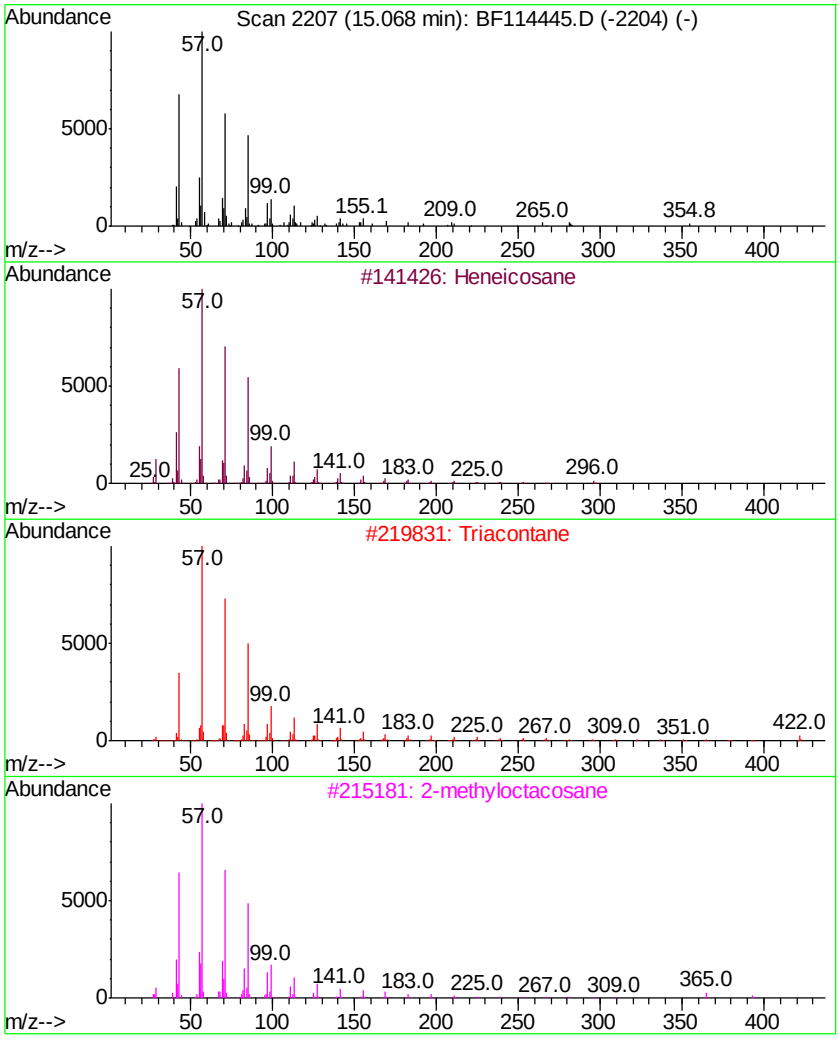
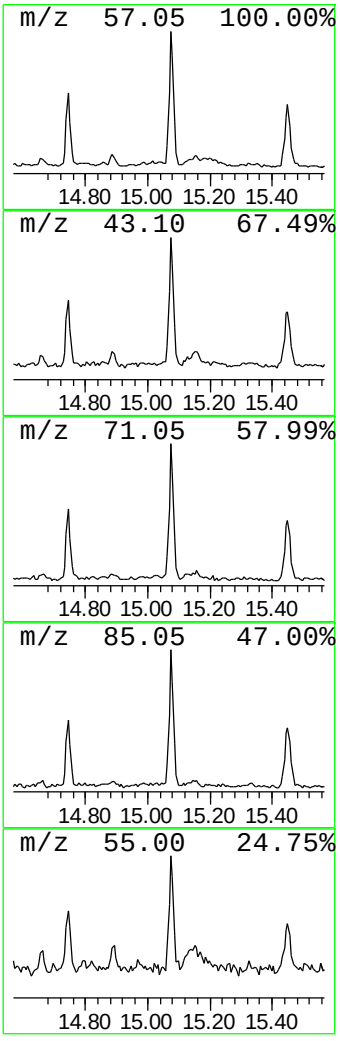
****

Peak Number 5 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.83 ng	211380	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Triacontane	422	C30H62	000638-68-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Docosane	310	C22H46	000629-97-0	87
5	Octadecane	254	C18H38	000593-45-3	87





Library Search Compound Report

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Operator : JU/SJ
Sample : K2943-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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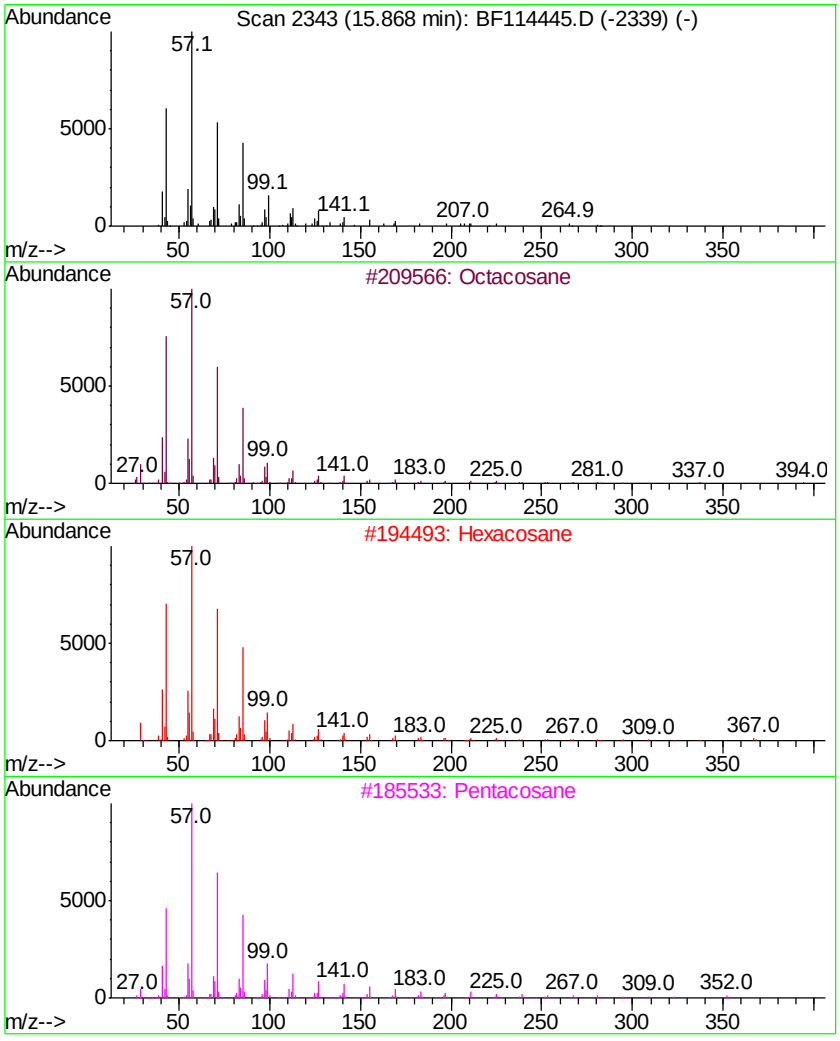
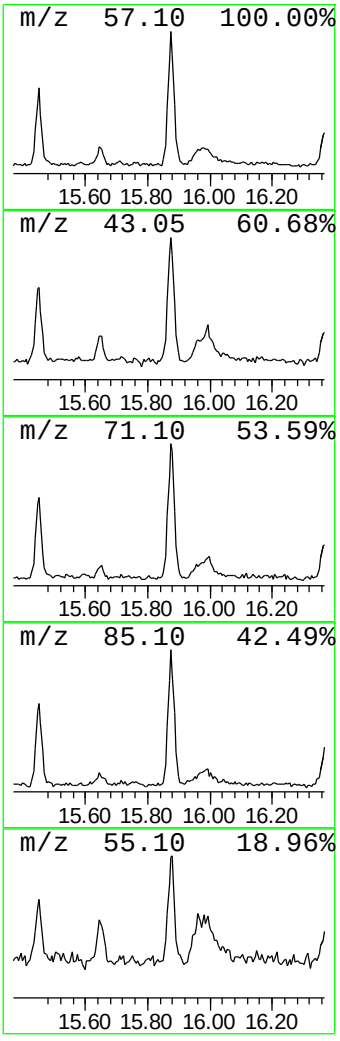
Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	3.04 ng	227193	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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Misc :
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Instrument : BNA_F
ClientSampleId : BUS-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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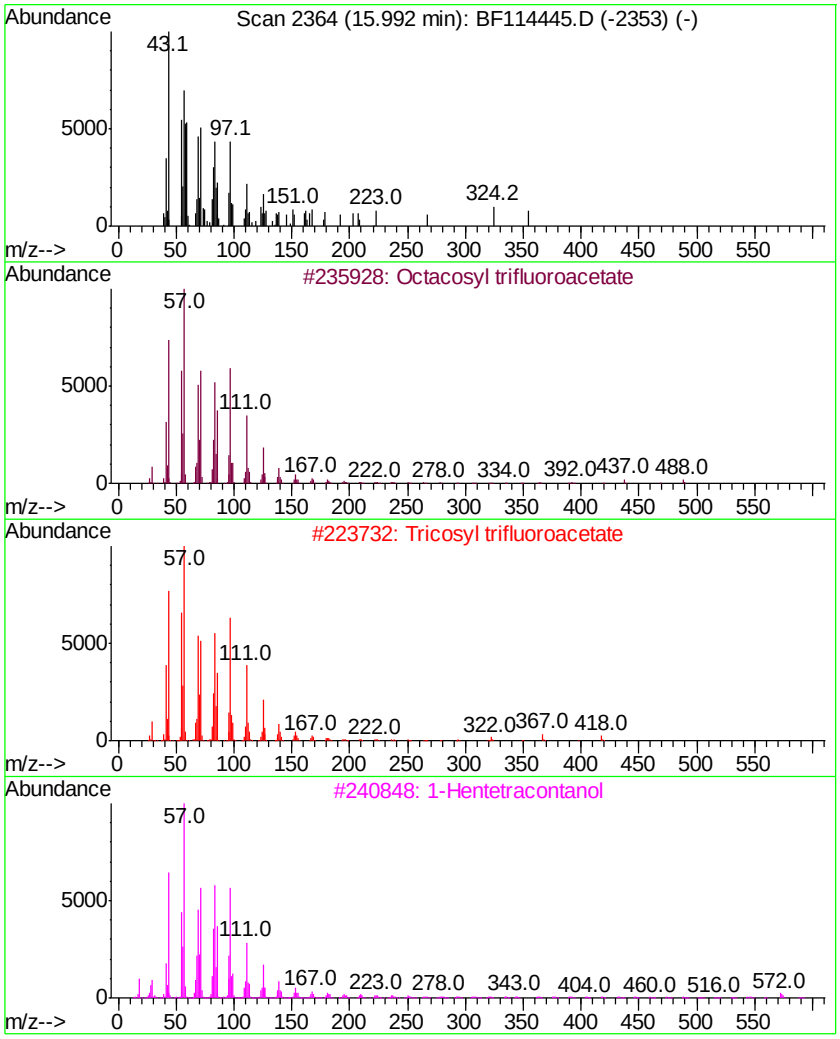
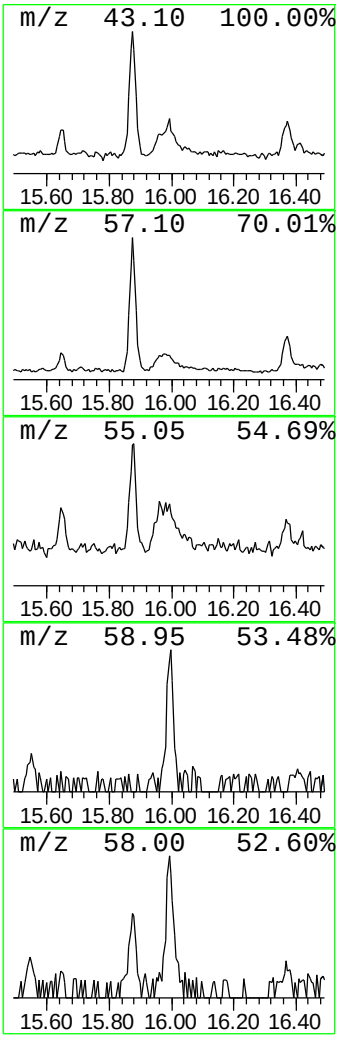
Peak Number 7 Octacosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.51 ng	187170	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	60
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	55
3	1-Hentetracontanol	593	C41H84O	040710-42-7	53
4	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	50
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	49





Tentatively Identified Compound (LSC) summary

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Data File : BF114445.D
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Misc :
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Instrument : BNA_F
ClientSampleId : BUS-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.60	6.60	89.3	ng	5056140	1	6.83	1132040	20.0
n-Hexadecanoic acid	11.87	5.6	ng	474551	4	11.35	1704600	20.0
Cycloeicosane	13.83	11.8	ng	897943	5	13.99	1521930	20.0
Heneicosane	15.07	2.8	ng	211380	6	15.46	1492600	20.0
Octacosane	15.87	3.0	ng	227193	6	15.46	1492600	20.0
Octacosyl trifluo...	15.99	2.5	ng	187170	6	15.46	1492600	20.0