LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052119\
Data File : BF114464.D
Acq On : 21 May 2019 18:57
Operator : JU/SJ
Sample : K2956-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FM5210

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	5.040	499	502	511	rVB	38686	52799	1.10%	0.143%
2	5.457	570	573	593	rVB	1949593	2111392	43.86%	5.706%
3	6.469	742	745	764	rBV	1229264	1498518	31.13%	4.049%
4	6.604	764	768	776	rBV	4023327	3649046	75.80%	9.861%
5	6.828	803	806	813	rBV	1470696	1232134	25.60%	3.330%
6	6.986	829	833	848	rVB	3807356	3359980	69.80%	9.080%
7	7.392	898	902	914	rBV	3008732	2784782	57.85%	7.525%
8	8.022	1005	1009	1018	rBV3	52897	125959	2.62%	0.340%
9	8.110	1021	1024	1040	rVB	1793604	1659270	34.47%	4.484%
10	9.186	1203	1207	1210	rBV	5521365	4813961	100.00%	13.009%
11	9.304	1222	1227	1230	rVB	105035	103602	2.15%	0.280%
12	9.527	1261	1265	1268	rBV	146628	115574	2.40%	0.312%
13	9.580	1271	1274	1278	rVV	190290	169718	3.53%	0.459%
14	9.869	1316	1323	1327	rBV	1873159	1827044	37.95%	4.937%
15	10.657	1453	1457	1471	rBV	2995104	2934506	60.96%	7.930%
16	11.239	1553	1556	1561	rBV2	95177	98541	2.05%	0.266%
17	11.351	1572	1575	1579	rBV	1846982	1748696	36.33%	4.726%
18	11.874	1661	1664	1675	rBV2	527819	569933	11.84%	1.540%
19	12.657	1794	1797	1809	rBV	204038	286526	5.95%	0.774%
20	12.933	1840	1844	1847	rBV	4266999	3853117	80.04%	10.412%
21	13.410	1920	1925	1929	rBV	72835	93564	1.94%	0.253%
22	13.833	1993	1997	2009	rBV5	102596	263527	5.47%	0.712%
23	13.998	2021	2025	2033	rBV	1176520	1206697	25.07%	3.261%
24	14.145	2047	2050	2052	rBV	72120	60142	1.25%	0.163%
25	14.445	2098	2101	2109	rBV	150350	154532	3.21%	0.418%
26	14.751	2149	2153	2156	rBV	180378	178341	3.70%	0.482%
27	15.080	2205	2209	2214	rBV	243335	258140	5.36%	0.698%
28	15.462	2269	2274	2286	rVB	961176	1405212	29.19%	3.797%
29	15.880	2341	2345	2351	rVB	171642	247781	5.15%	0.670%
30	16.374	2425	2429	2434	rVB	87783	142019	2.95%	0.384%

Sum of corrected areas: 37005053

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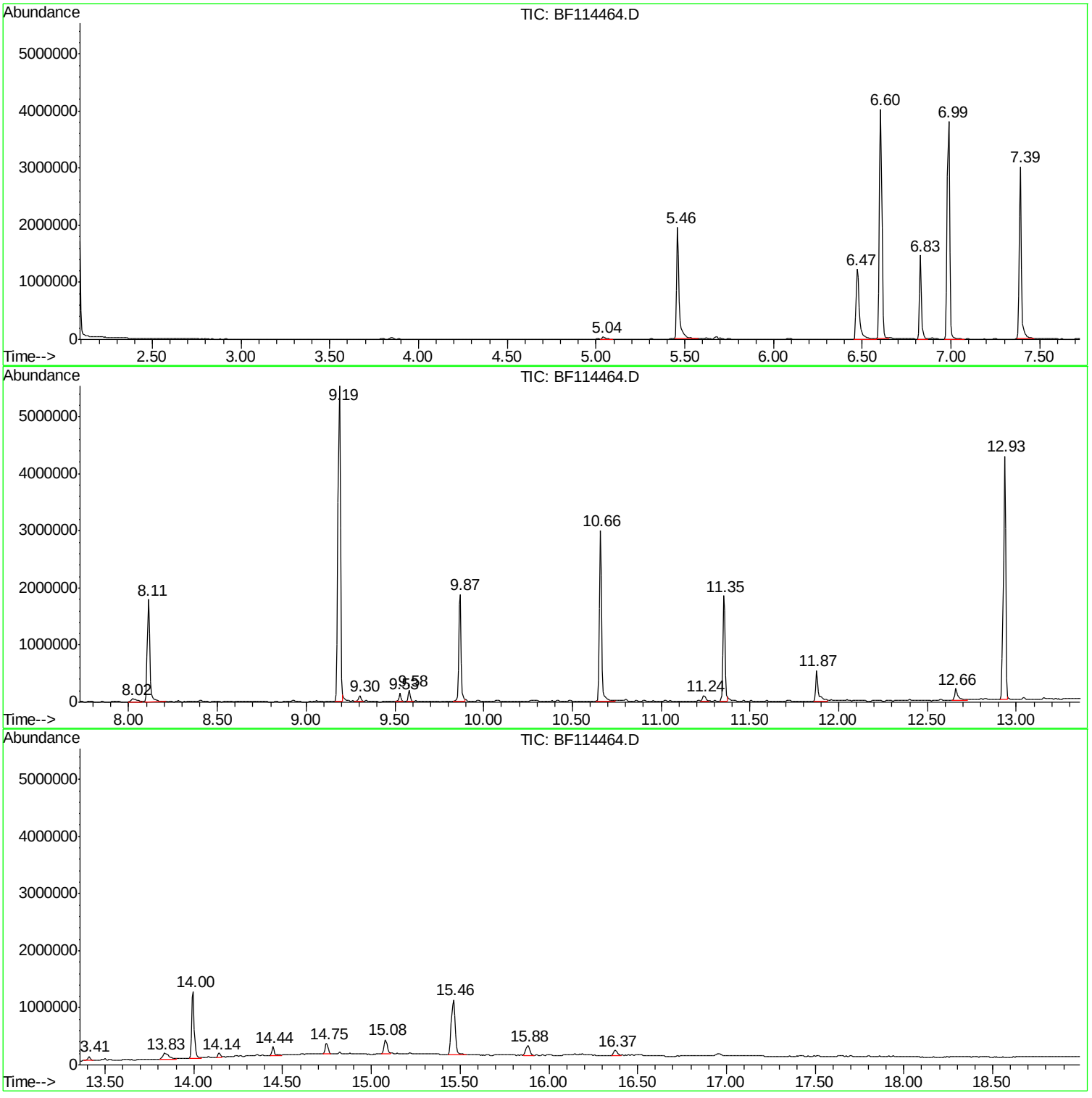
Acq On : 21 May 2019 18:57
Operator : JU/SJ
Sample : K2956-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FM5210

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



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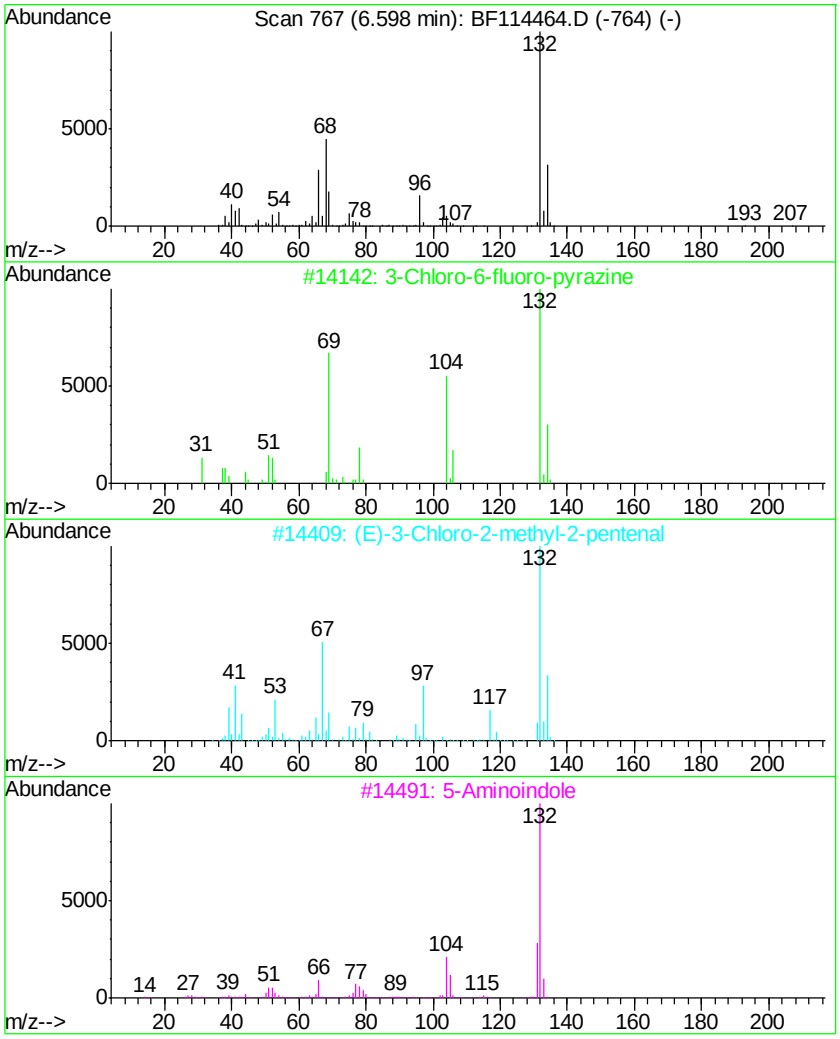
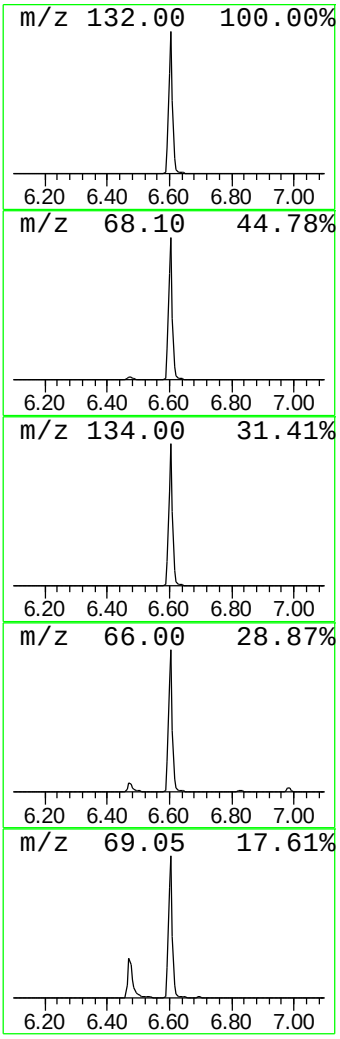
****

Peak Number 1 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	59.23 ng	3649050	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Data File : BF114464.D
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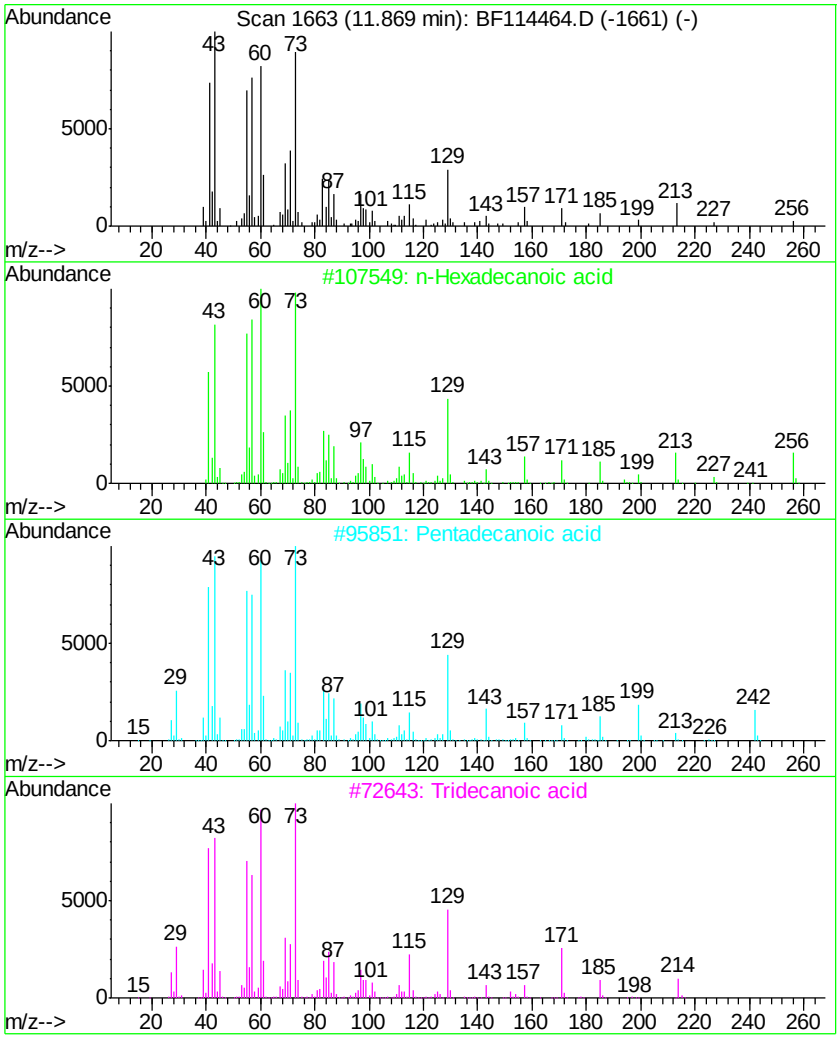
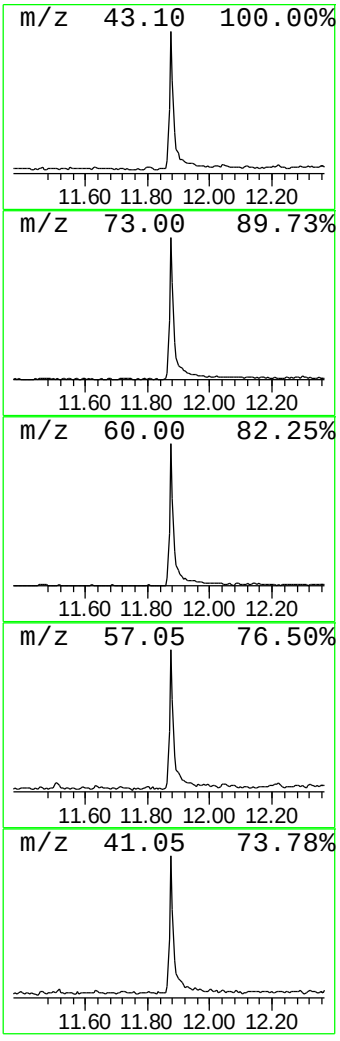
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	6.52 ng	569933	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Misc :
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Instrument : BNA_F
ClientSampleId : FM5210

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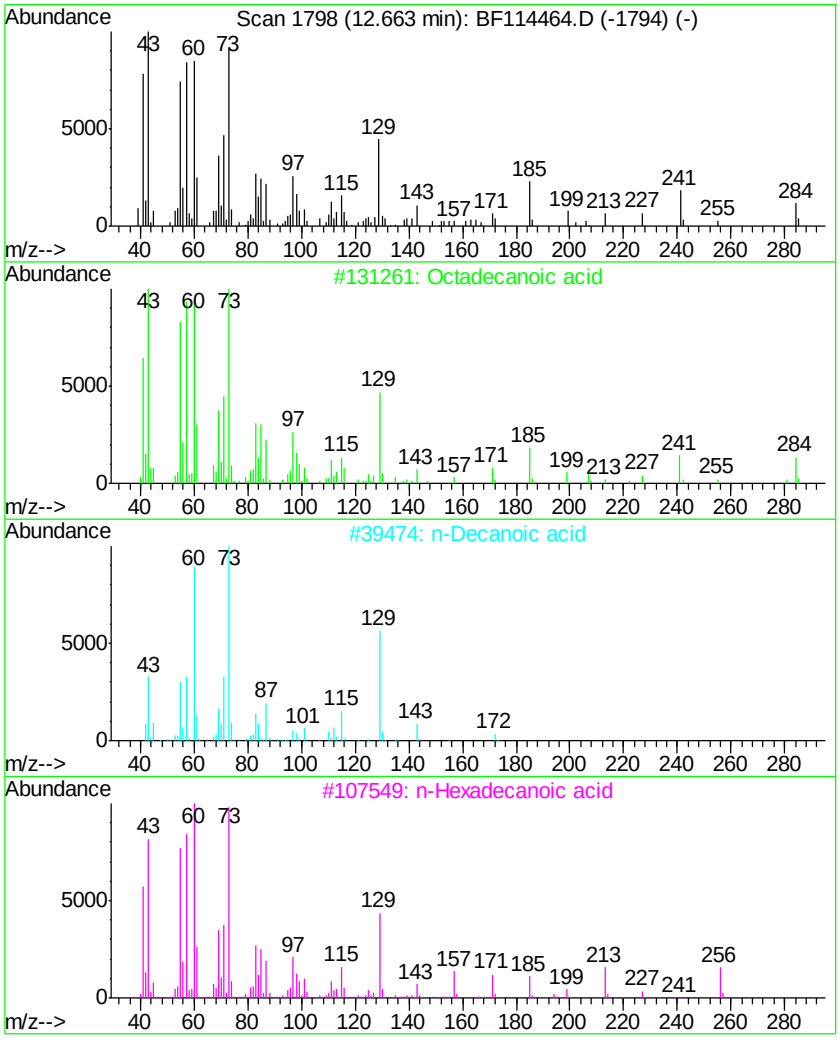
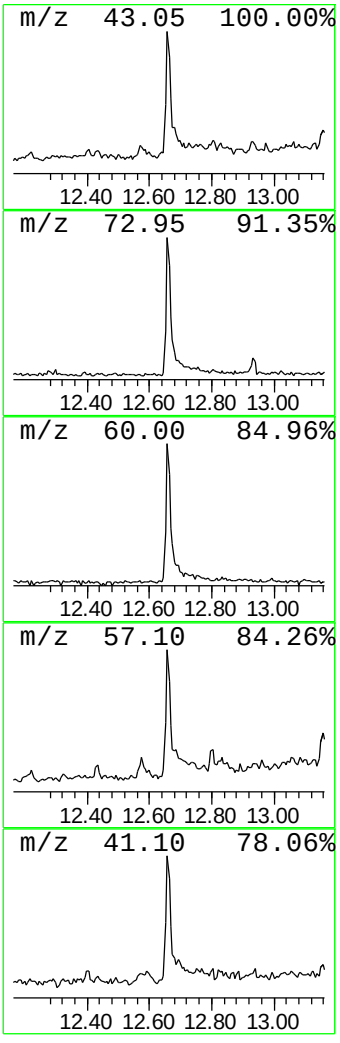
****

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	3.28 ng	286526	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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Misc :
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Instrument : BNA_F
ClientSampleId : FM5210

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
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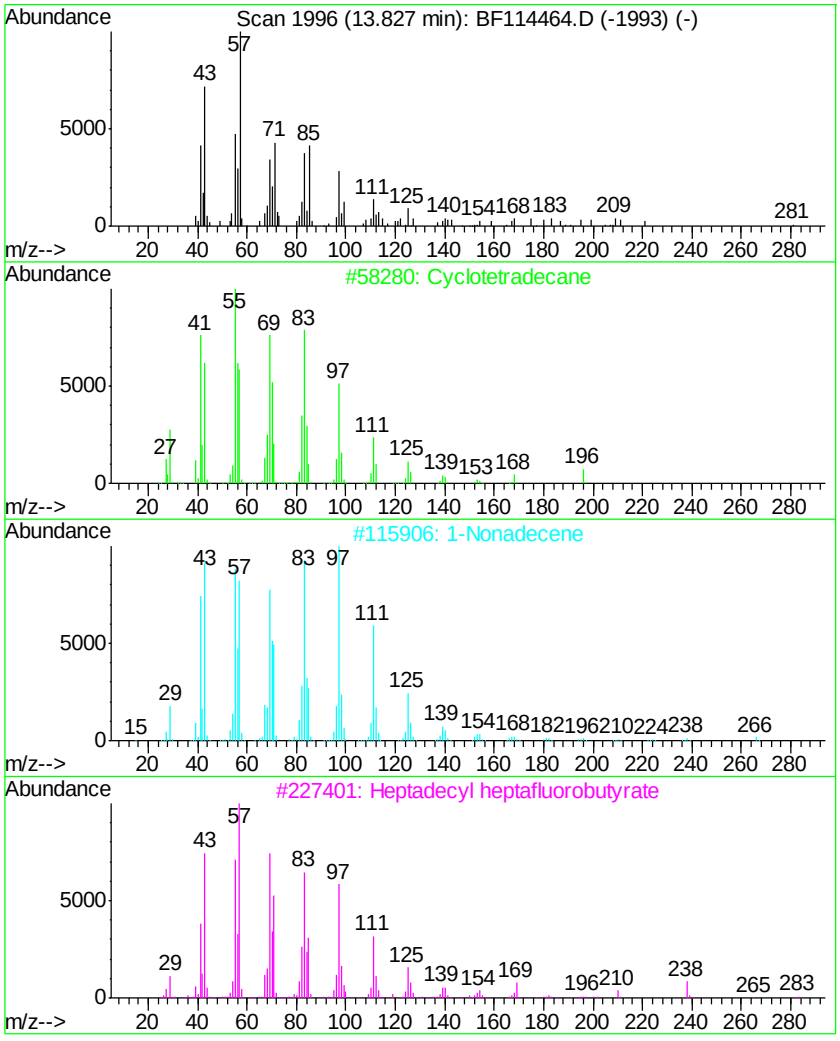
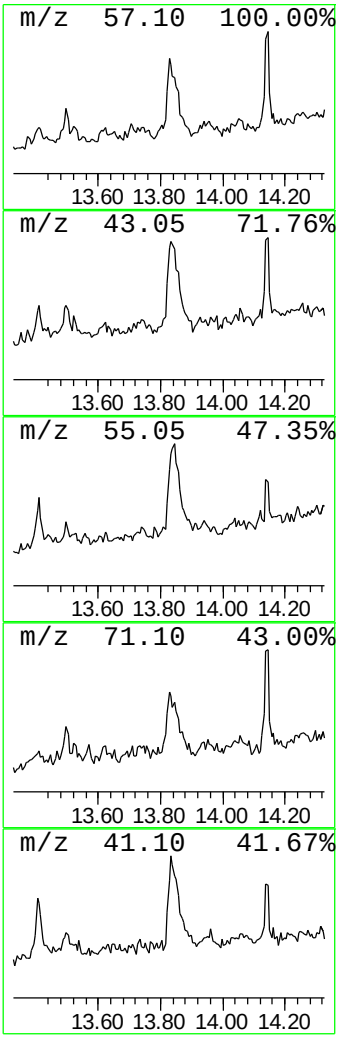
****

Peak Number 5 Cyclotetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.37 ng	263527	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	95
2	1-Nonadecene	266	C19H38	018435-45-5	90
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	89
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	76
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	76





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Misc :
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Instrument : BNA_F
ClientSampleId : FM5210

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TIC Library : C:\DATABASE\NIST11.L
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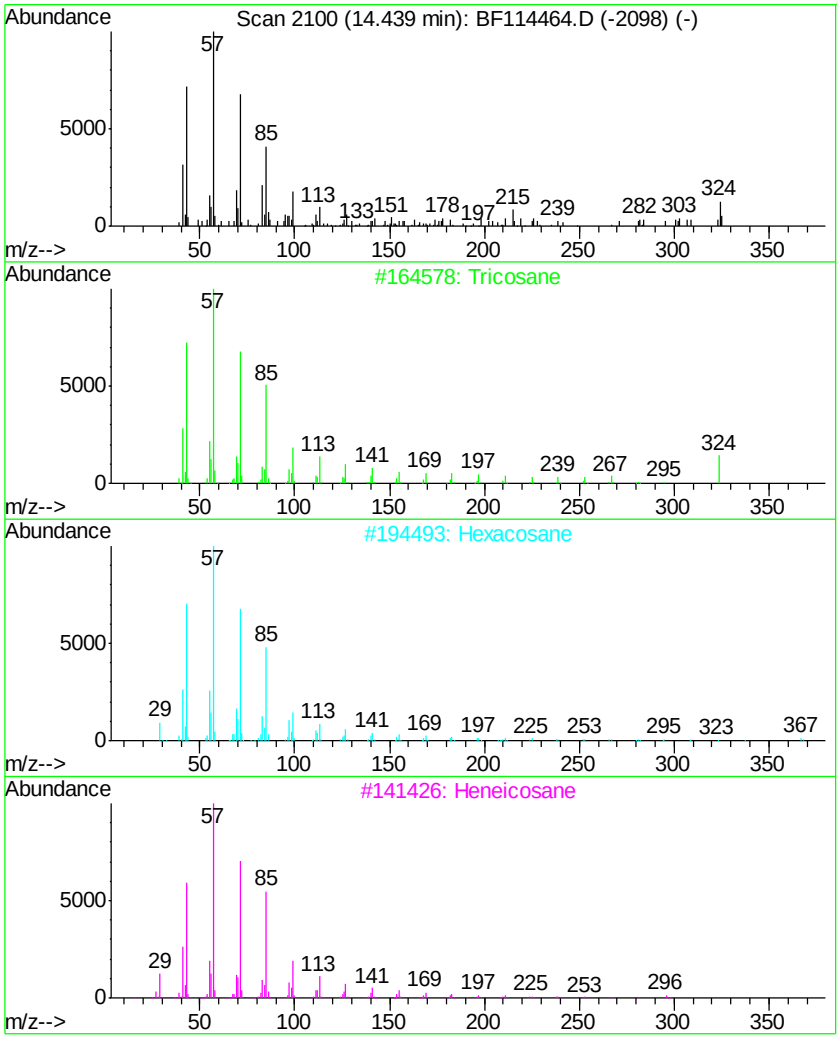
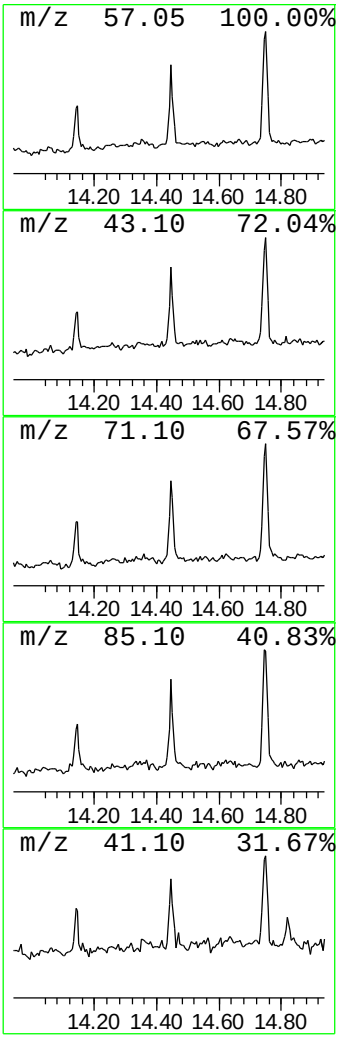
****

Peak Number 6 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.56 ng	154532	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Nonadecane	268	C19H40	000629-92-5	83





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
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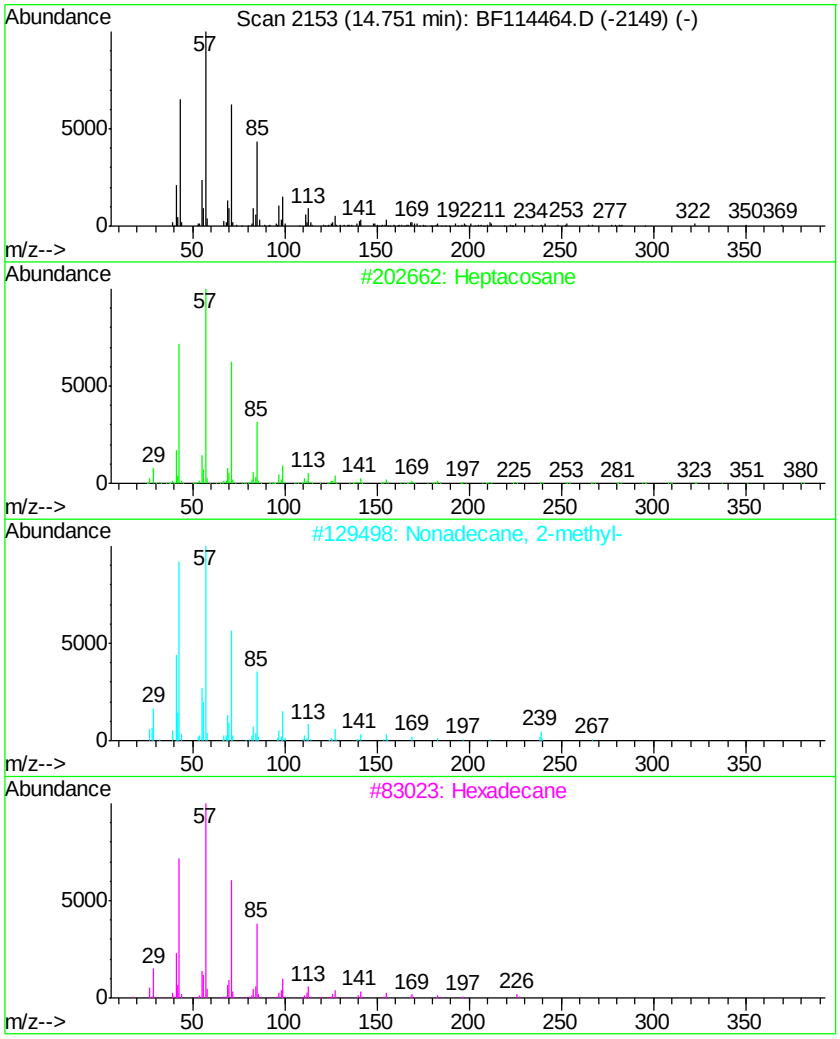
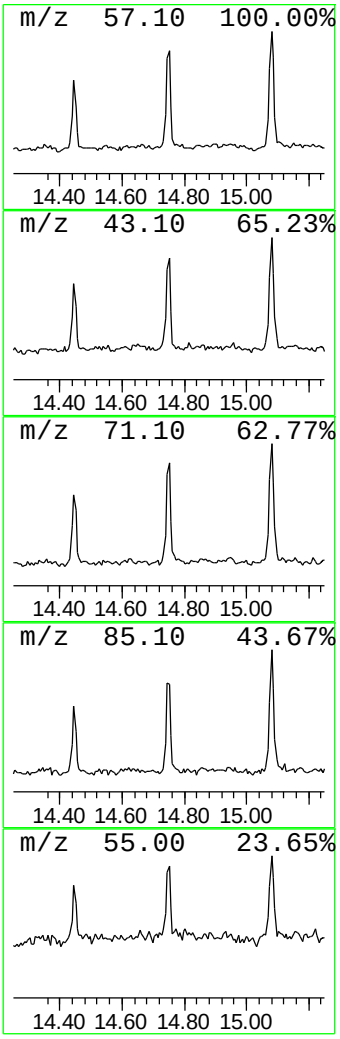
****

Peak Number 7 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.54 ng	178341	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
3	Hexadecane	226	C16H34	000544-76-3	83
4	Heneicosane	296	C21H44	000629-94-7	72
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	70





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

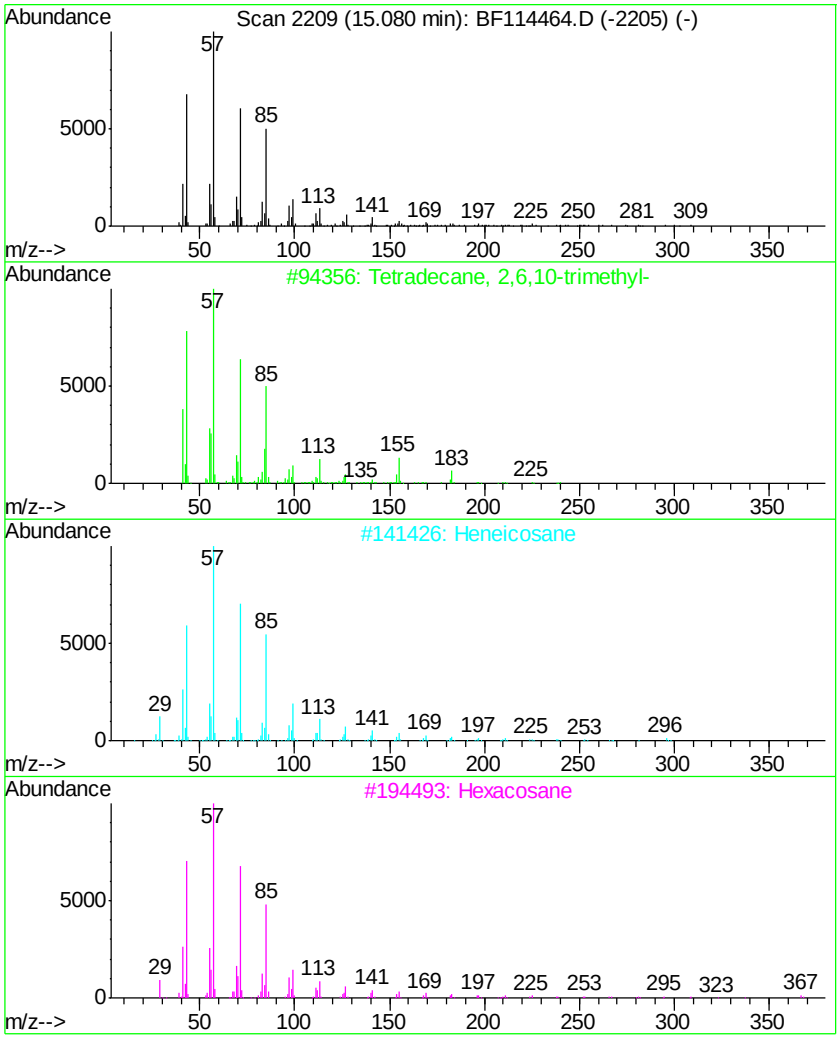
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

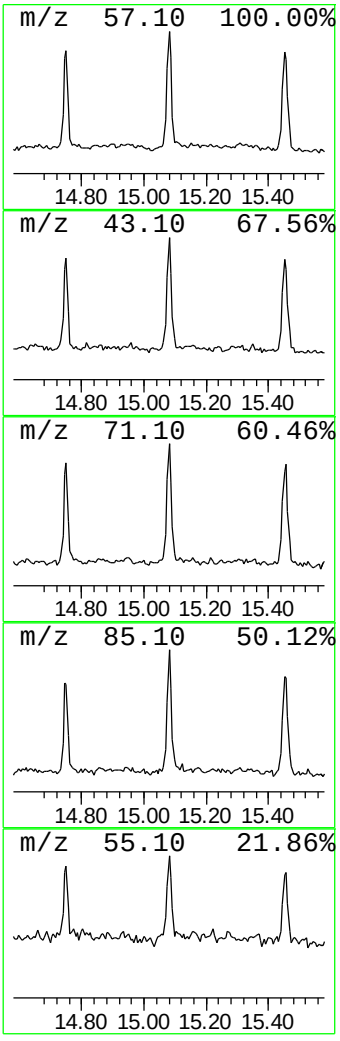
****

Peak Number 8 Tetradecane, 2,6,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	3.67 ng	258140	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Octadecane	254	C18H38	000593-45-3	90





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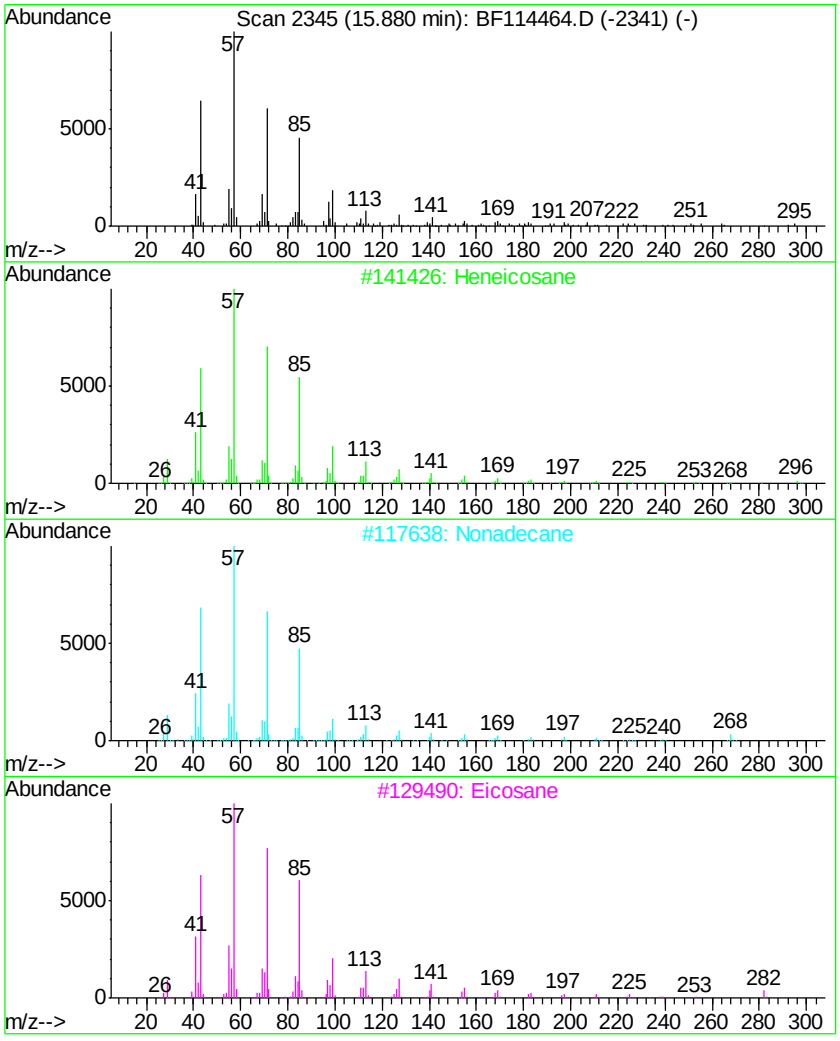
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

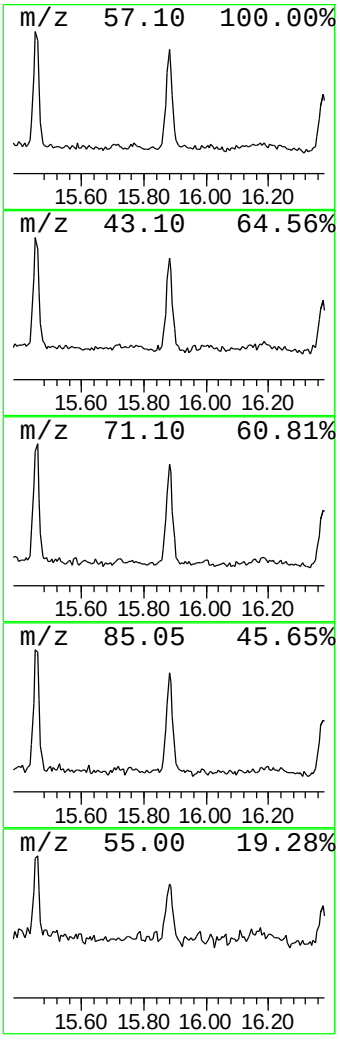
****

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	3.53 ng	247781	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	72
2	Nonadecane	268	C19H40	000629-92-5	72
3	Eicosane	282	C20H42	000112-95-8	72
4	Heptadecane	240	C17H36	000629-78-7	72
5	Octadecane	254	C18H38	000593-45-3	72





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Instrument : BNA_F
ClientSampleId : FM5210

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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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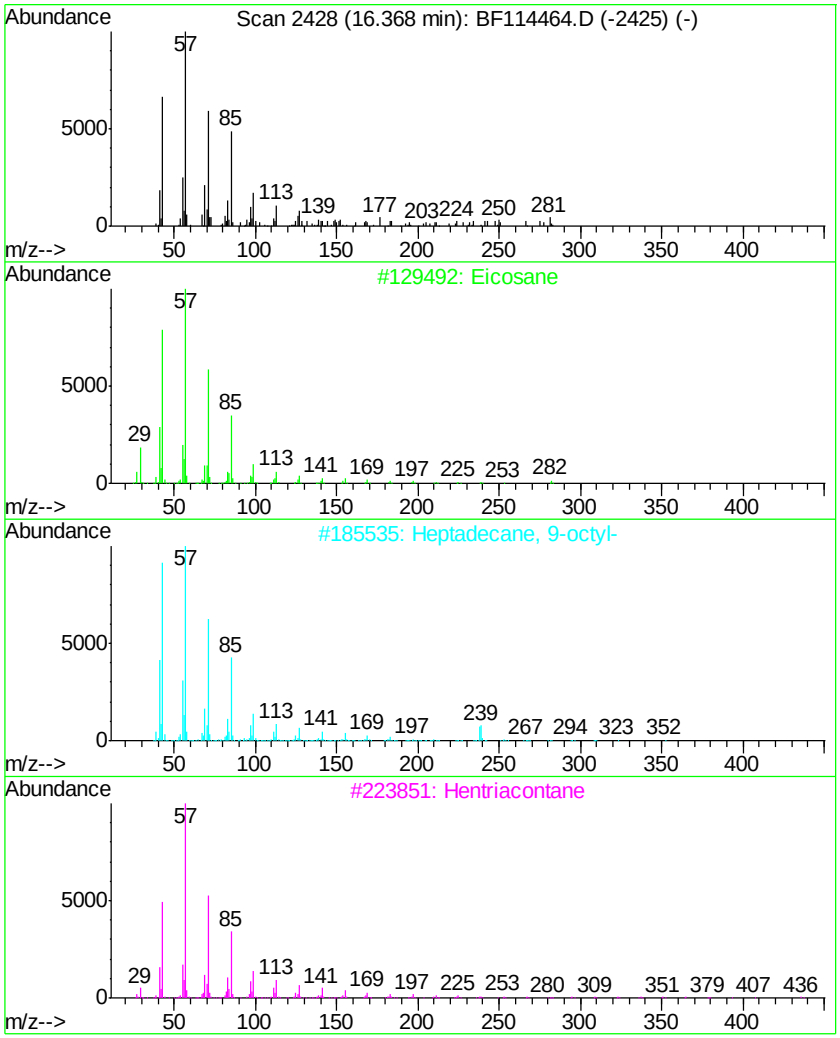
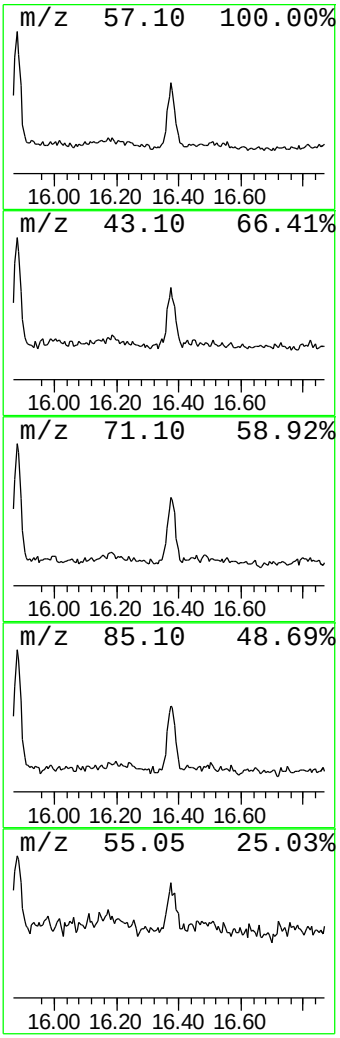
Peak Number 10 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	2.02 ng	142019	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
3	Hentriacontane	437	C31H64	000630-04-6	83
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	80
5	Tetradecane	198	C14H30	000629-59-4	80





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_F
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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	59.2	ng	3649050	1	6.83	1232130	20.0
n-Hexadecanoic acid	11.87	6.5	ng	569933	4	11.35	1748700	20.0
Octadecanoic acid	12.66	3.3	ng	286526	4	11.35	1748700	20.0
Cyclotetradecane	13.83	4.4	ng	263527	5	14.00	1206700	20.0
Tricosane	14.44	2.6	ng	154532	5	14.00	1206700	20.0
Heptacosane	14.75	2.5	ng	178341	6	15.46	1405210	20.0
Tetradecane, 2,6,...	15.08	3.7	ng	258140	6	15.46	1405210	20.0
Heneicosane	15.88	3.5	ng	247781	6	15.46	1405210	20.0
Eicosane	16.37	2.0	ng	142019	6	15.46	1405210	20.0