LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
Data File : BF100742.D
Acq On : 20 Nov 2017 20:46
Operator : SJ/JU
Sample : I6521-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	5.110	510	514	524	rBV	126190	184619	6.83%	0.775%
2	5.493	573	579	582	rBV	2223015	2376995	87.89%	9.984%
3	6.504	744	751	755	rBV	1965097	2488574	92.02%	10.453%
4	6.645	769	775	778	rBV	2242253	2463996	91.11%	10.349%
5	6.869	810	813	817	rVB	686786	548208	20.27%	2.303%
6	7.028	835	840	843	rBV	2136304	1913062	70.74%	8.035%
7	7.434	903	909	912	rBV	1478593	1590810	58.82%	6.682%
8	7.898	984	988	990	rVB	71657	64213	2.37%	0.270%
9	8.151	1027	1031	1034	rBV	898681	723547	26.75%	3.039%
10	9.228	1208	1214	1217	rBV	2937077	2704360	100.00%	11.359%
11	9.298	1223	1226	1229	rBV	42522	35026	1.30%	0.147%
12	9.616	1277	1280	1283	rBV	212656	166808	6.17%	0.701%
13	9.828	1313	1316	1320	rVB	103744	79646	2.95%	0.335%
14	9.904	1325	1329	1333	rVB	850344	782730	28.94%	3.288%
15	10.328	1399	1401	1404	rVB	110795	84193	3.11%	0.354%
16	10.551	1434	1439	1441	rBV	28603	35746	1.32%	0.150%
17	10.698	1459	1464	1467	rBV	1525358	1462918	54.09%	6.145%
18	10.804	1478	1482	1487	rBV	78604	93712	3.47%	0.394%
19	11.251	1552	1558	1560	rBV2	36300	35176	1.30%	0.148%
20	11.392	1578	1582	1584	rBV	901043	734079	27.14%	3.083%
21	11.416	1584	1586	1589	rVB	119817	90228	3.34%	0.379%
22	11.892	1663	1667	1668	rBV	31675	32285	1.19%	0.136%
23	11.910	1668	1670	1674	rVB2	96469	100737	3.72%	0.423%
24	12.004	1683	1686	1688	rBV2	46596	47466	1.76%	0.199%
25	12.439	1756	1760	1763	rBV	29733	35802	1.32%	0.150%
26	12.604	1784	1788	1791	rBV	255644	215615	7.97%	0.906%
27	12.692	1800	1803	1807	rBV2	41960	37441	1.38%	0.157%
28	12.833	1821	1827	1833	rBV	238658	256948	9.50%	1.079%
29	12.974	1847	1851	1854	rBV	1921032	1799809	66.55%	7.560%
30	13.051	1859	1864	1867	rBV3	23828	40137	1.48%	0.169%
31	13.157	1880	1882	1885	rVB	48377	40099	1.48%	0.168%
32	13.263	1896	1900	1903	rBV2	36705	34775	1.29%	0.146%
33	13.757	1980	1984	1986	rBV	60435	59233	2.19%	0.249%
34	13.863	1999	2002	2012	rVB2	86342	117741	4.35%	0.495%

LSC Area Percent Report

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Sample : I6521-05
Misc :
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Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.027	2026	2030	2033	rVV2	552693	543957	20.11%	2.285%
36	14.051	2033	2034	2040	rVB	121284	100596	3.72%	0.423%
37	14.127	2042	2047	2050	rBV4	30545	47206	1.75%	0.198%
38	14.410	2091	2095	2098	rBV	33860	38803	1.43%	0.163%
39	14.504	2106	2111	2114	rBV5	19932	37727	1.40%	0.158%
40	15.068	2203	2207	2214	rBV	124806	230625	8.53%	0.969%
41	15.374	2255	2259	2264	rVB	84151	111541	4.12%	0.469%
42	15.433	2265	2269	2275	rVV	114554	155503	5.75%	0.653%
43	15.504	2275	2281	2292	rVV	466322	659837	24.40%	2.772%
44	16.204	2398	2400	2407	rVB8	19541	31914	1.18%	0.134%
45	16.645	2469	2475	2486	rVB9	24972	56041	2.07%	0.235%
46	16.968	2524	2530	2539	rVB2	62505	125995	4.66%	0.529%
47	17.151	2557	2561	2566	rVB4	18156	28409	1.05%	0.119%
48	17.215	2566	2572	2578	rBV6	15946	40858	1.51%	0.172%
49	17.415	2599	2606	2616	rBV2	53634	122147	4.52%	0.513%

Sum of corrected areas: 23807893

LSC Report - Integrated Chromatogram

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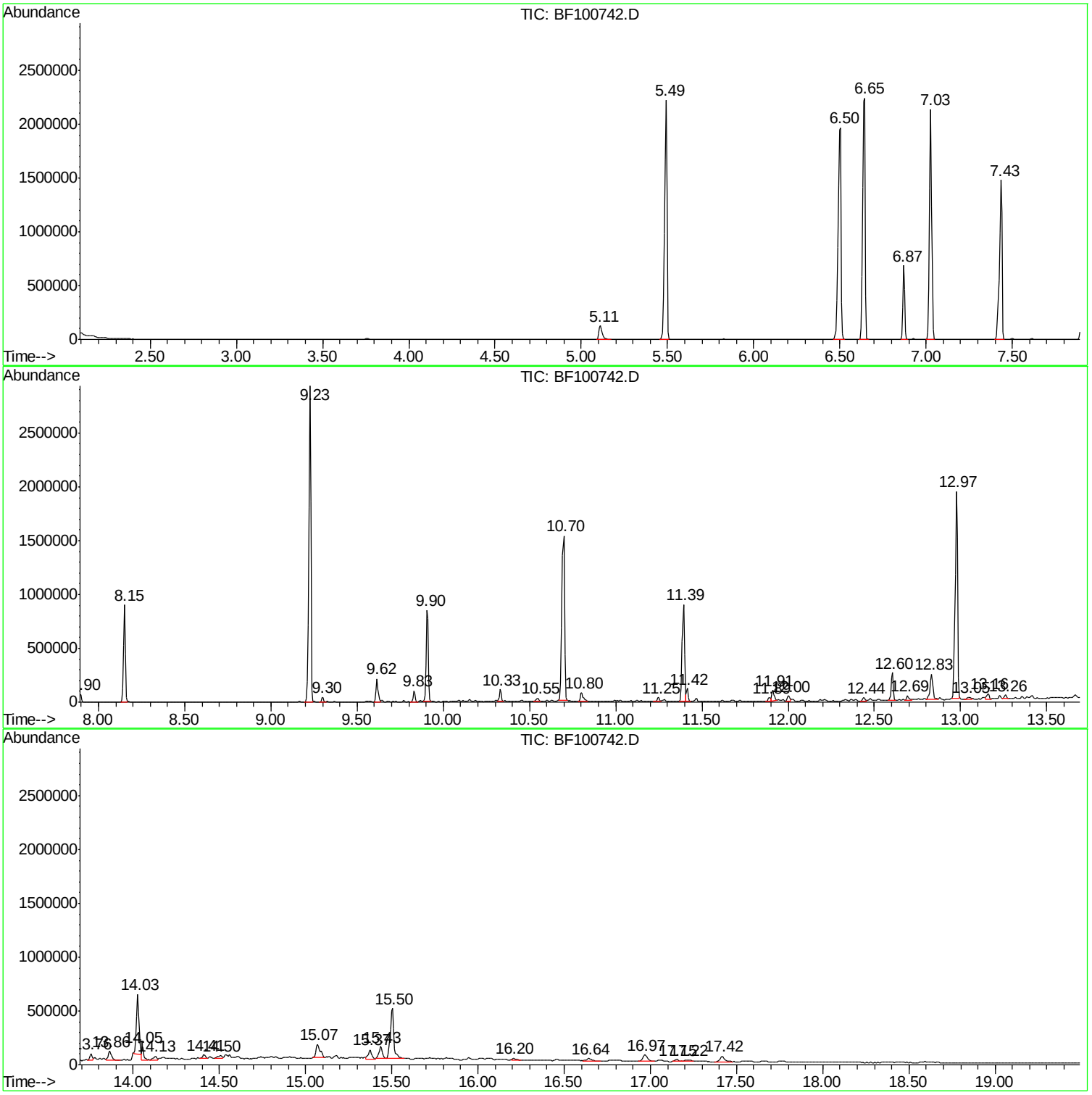
Sample : I6521-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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Operator : SJ/JU
Sample : I6521-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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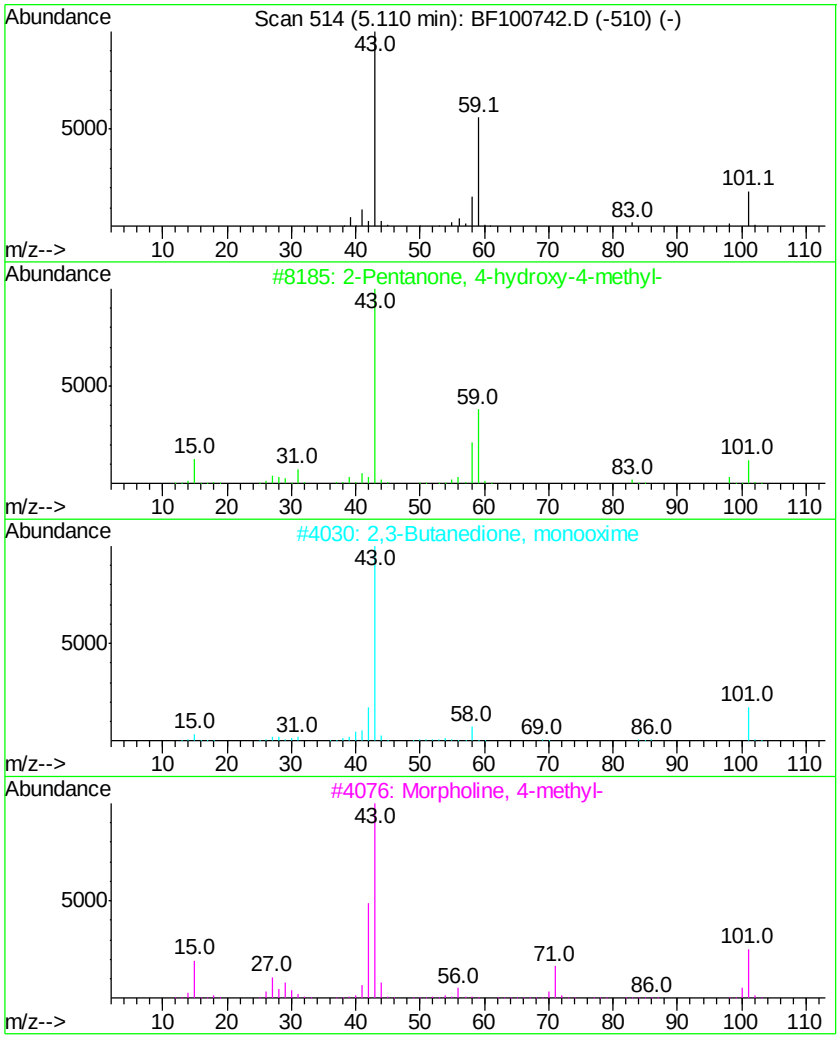
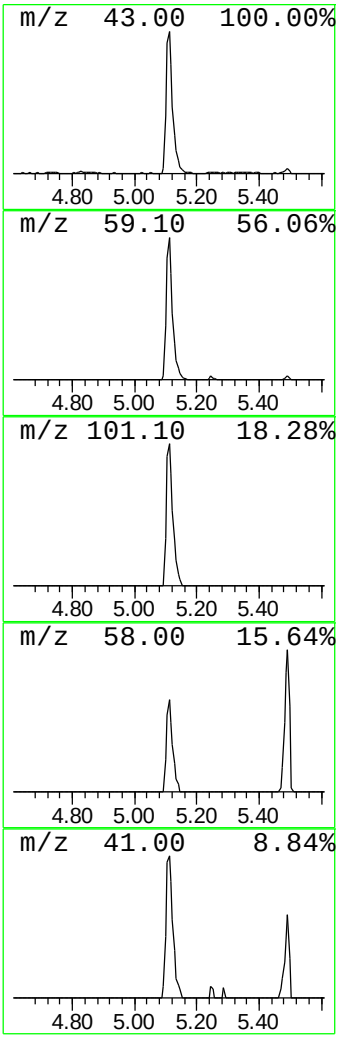
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	6.74 ng	184619	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
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Sample : I6521-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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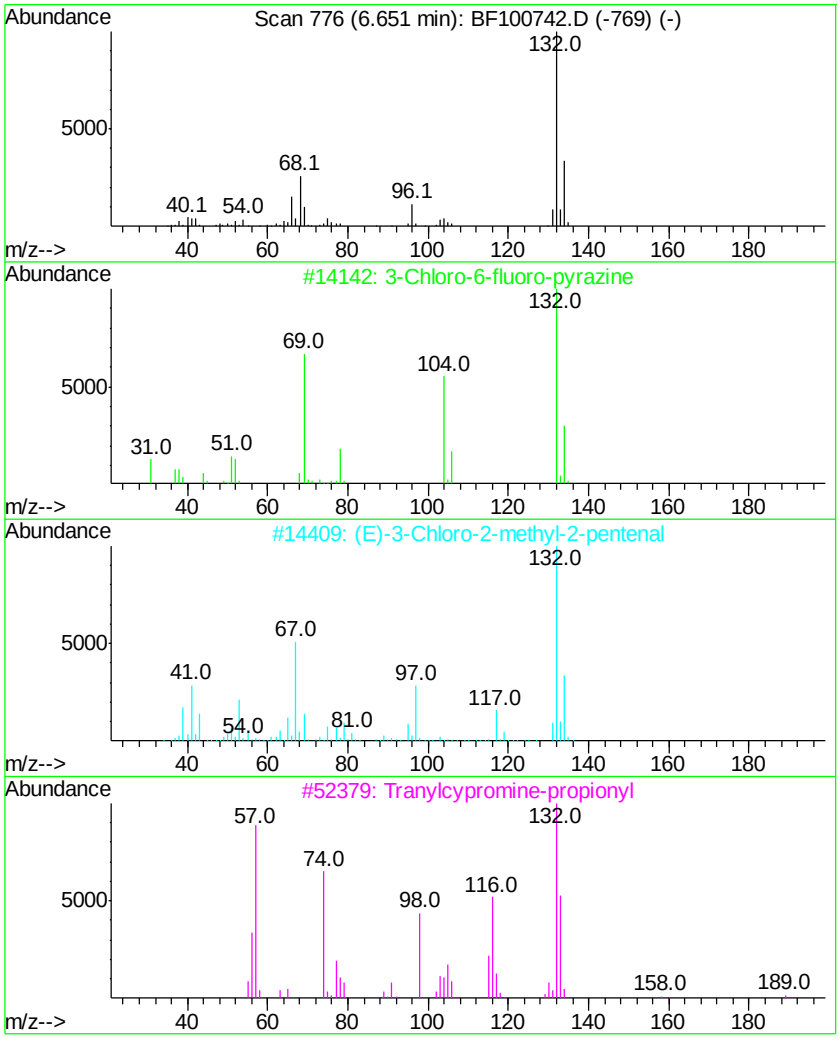
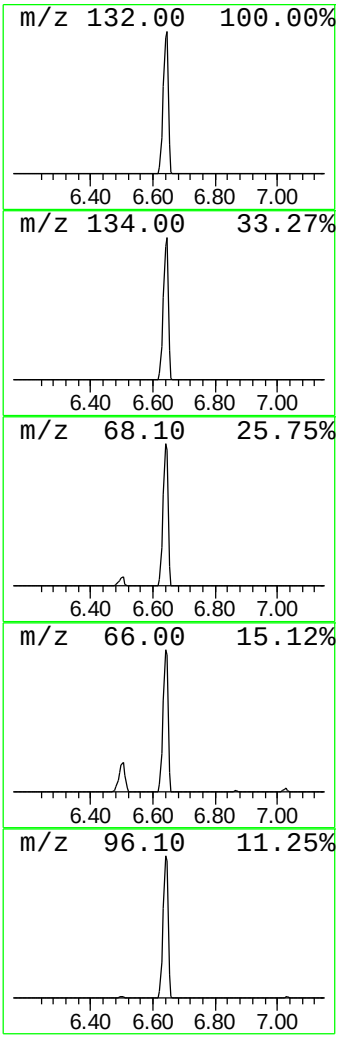
Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	89.89 ng	2464000	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : I6521-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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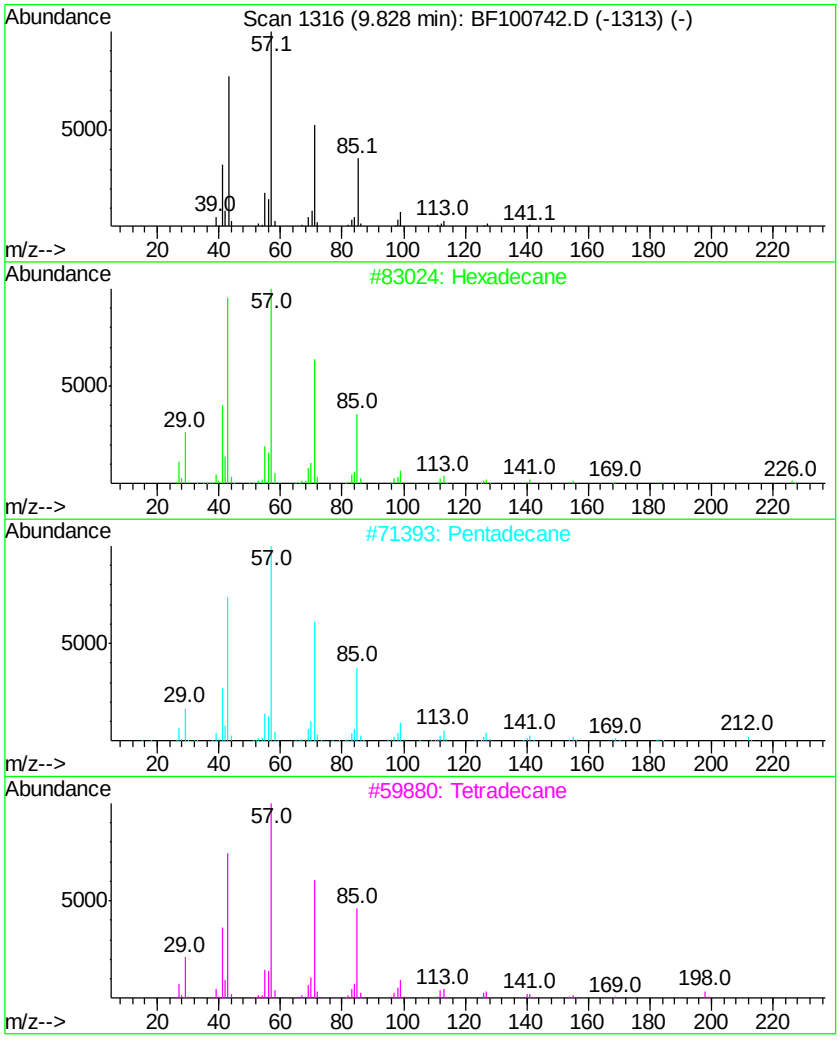
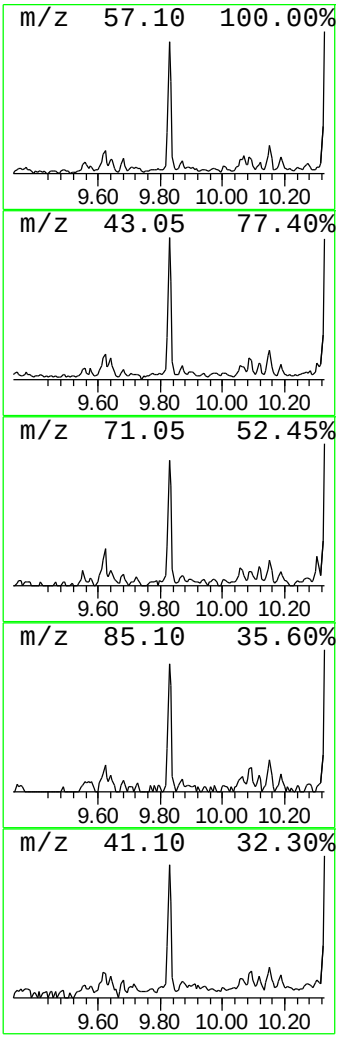
Peak Number 4 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.04 ng	79646	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Pentadecane	212	C15H32	000629-62-9	90
3	Tetradecane	198	C14H30	000629-59-4	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Heptadecane	240	C17H36	000629-78-7	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
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Operator : SJ/JU
Sample : I6521-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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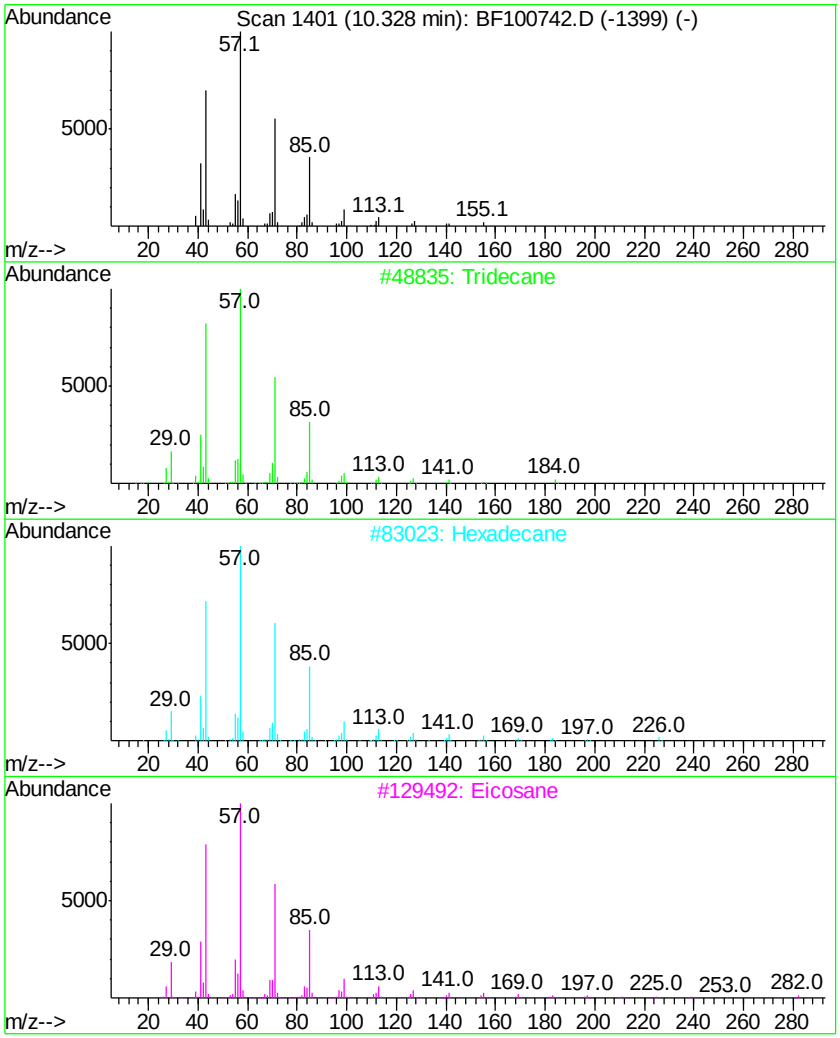
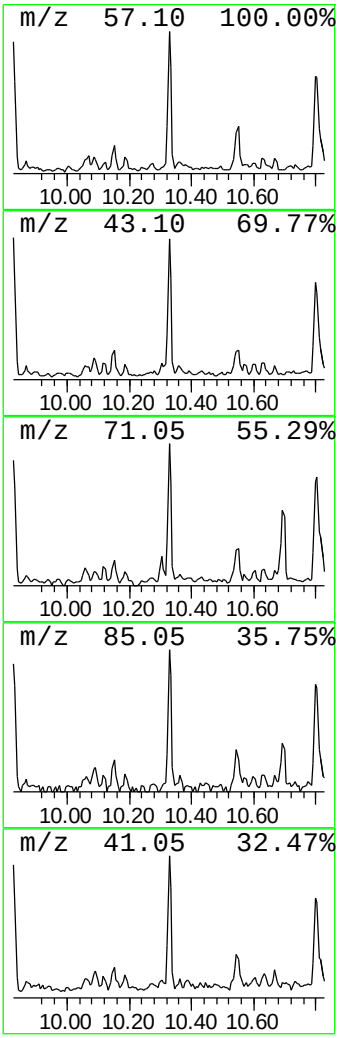
Peak Number 5 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.15 ng	84193	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Tetradecane	198	C14H30	000629-59-4	86
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	72





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Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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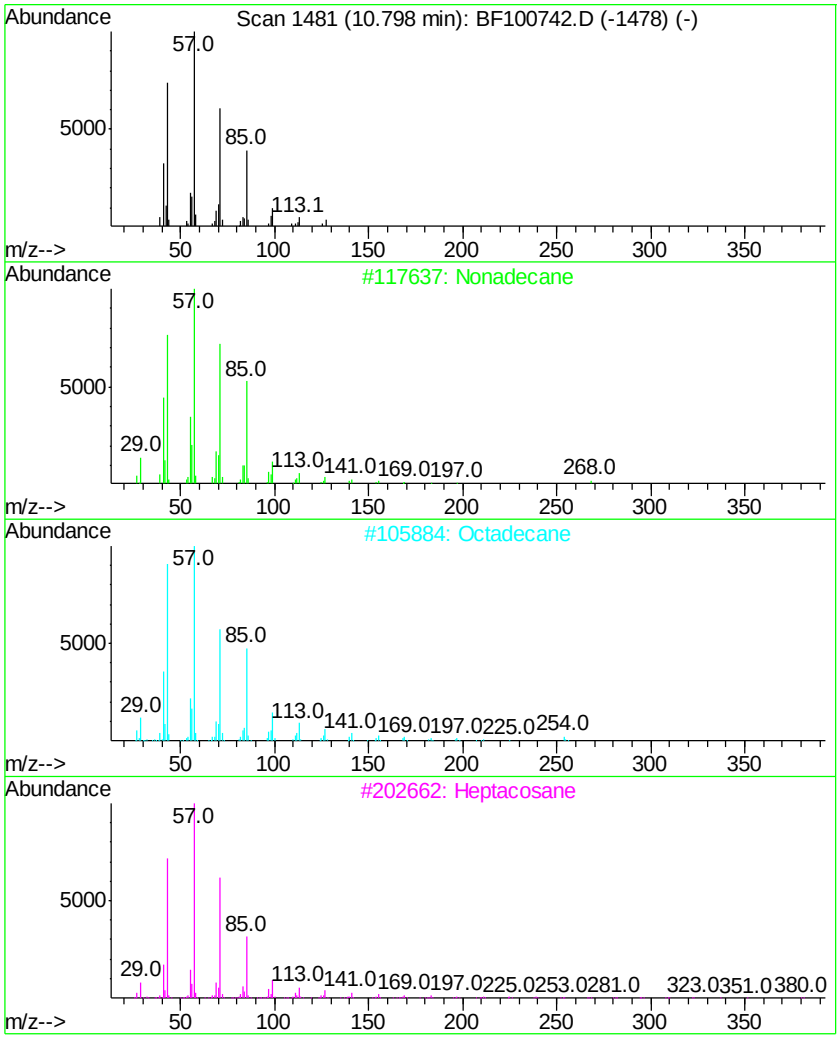
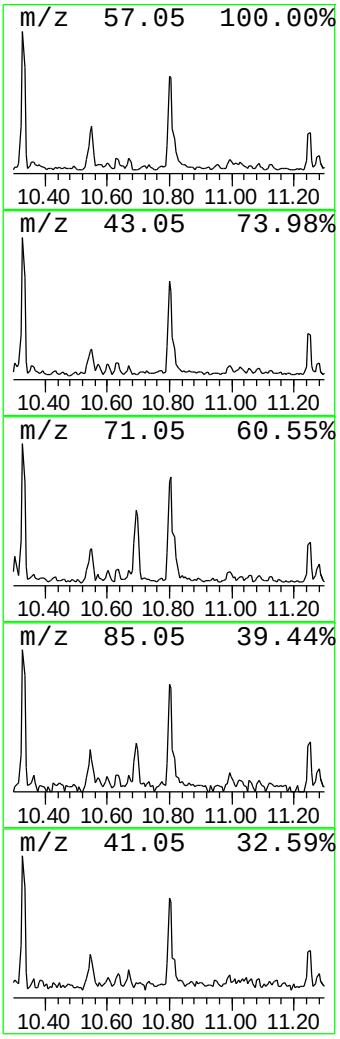
Peak Number 6 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.55 ng	93712	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Eicosane	282	C20H42	000112-95-8	90
5	Tetradecane	198	C14H30	000629-59-4	90





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ClientSampleId : TP-1-(0-5)

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TIC Library : C:\DATABASE\NIST11.L
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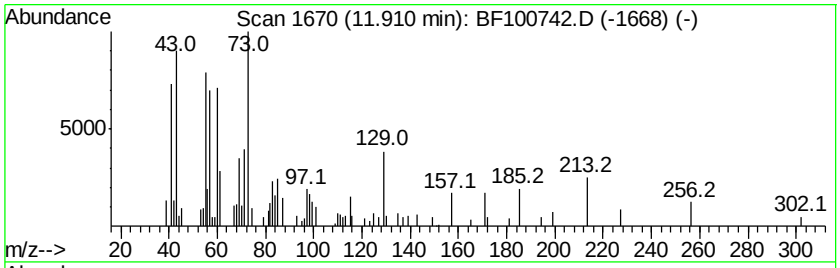
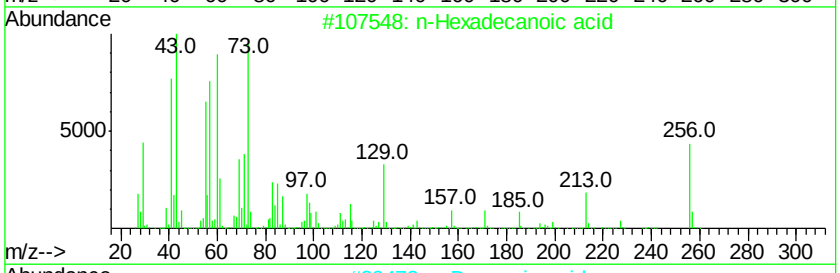
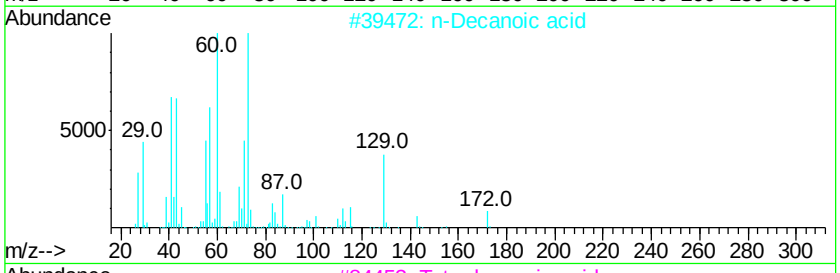
Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

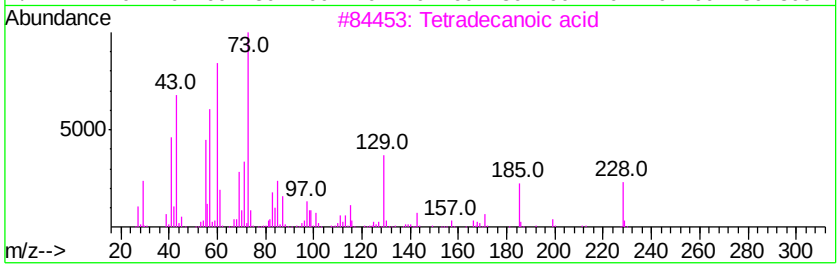
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.74 ng	100737	Phenanthrene-d10	11.39

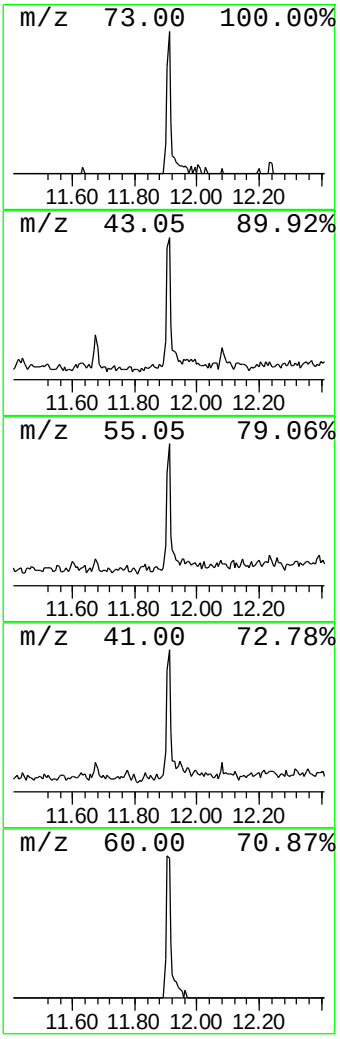
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	n-Decanoic acid	172	C10H20O2	000334-48-5	60
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	47











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ClientSampleId : TP-1-(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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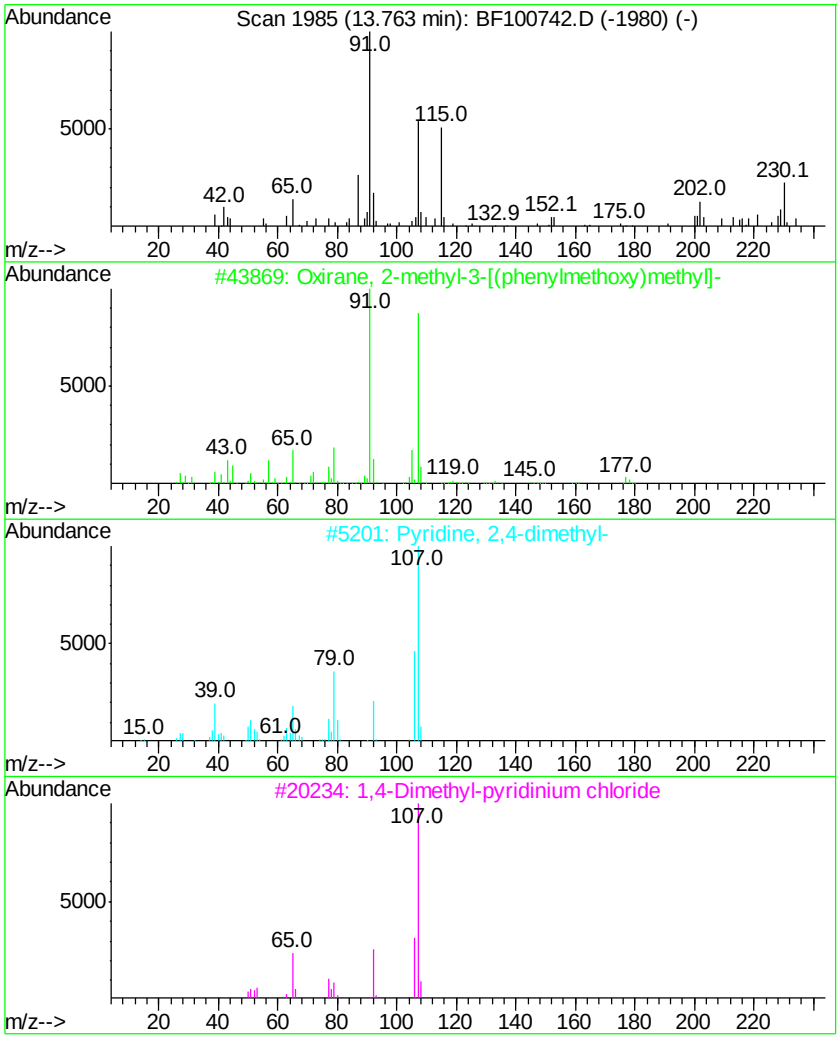
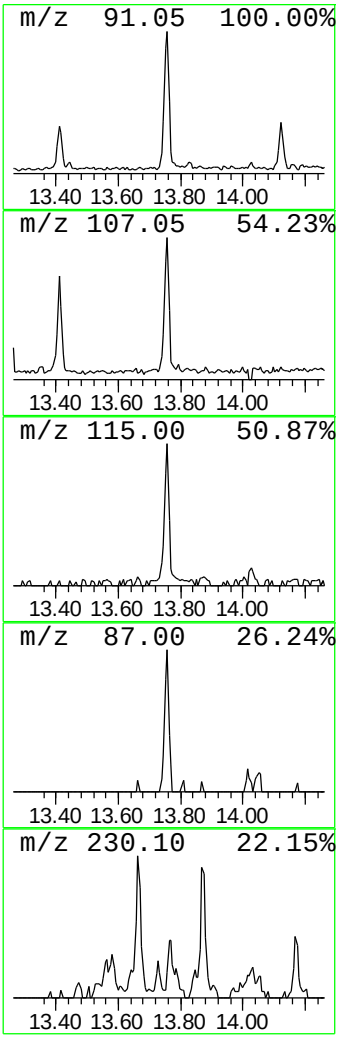
Peak Number 8 unknown13.76 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	2.18 ng	59233	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, 2-methyl-3-[(phenylmeth...	178	C11H14O2	116296-88-9	38
2	Pyridine, 2,4-dimethyl-	107	C7H9N	000108-47-4	22
3	1,4-Dimethyl-pyridinium chloride	143	C7H10ClN	1000145-43-8	22
4	Benzeneacetic acid, 4-hydroxy-	152	C8H8O3	000156-38-7	18
5	1-[(Pyrazinylcarbonyl)oxy]-2,5-p...	221	C9H7N3O4	342612-63-9	14





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Integration Parameters: LSCINT.P

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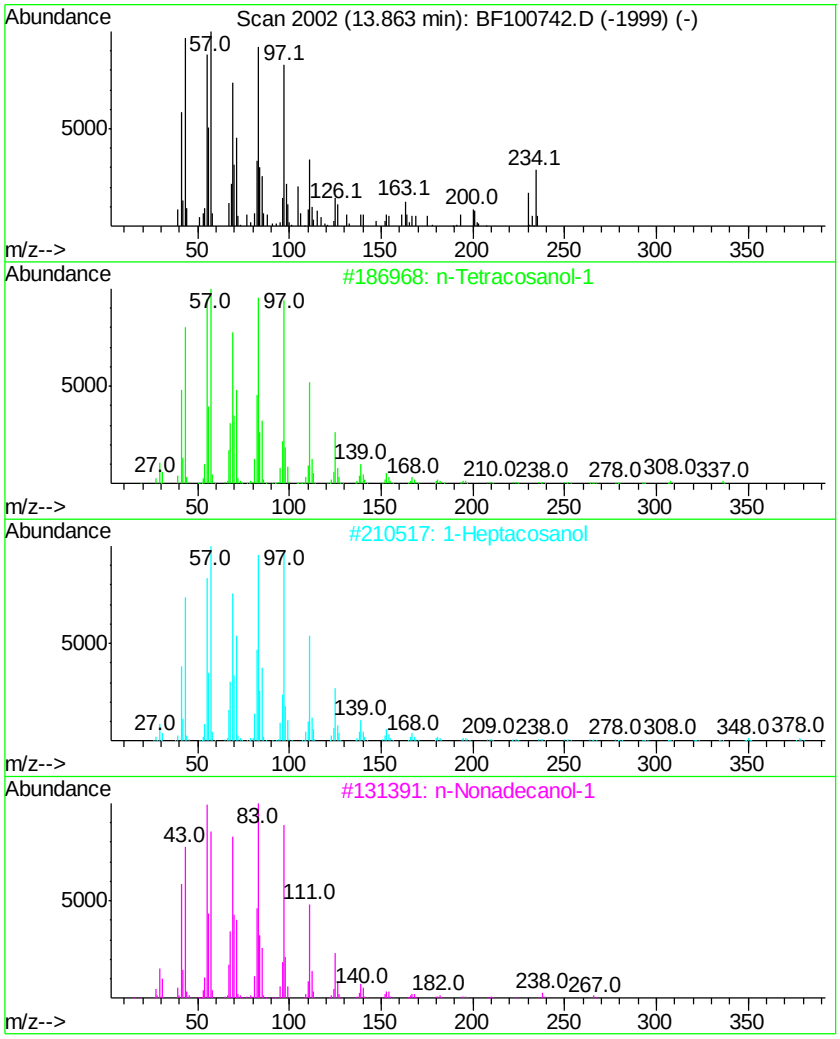
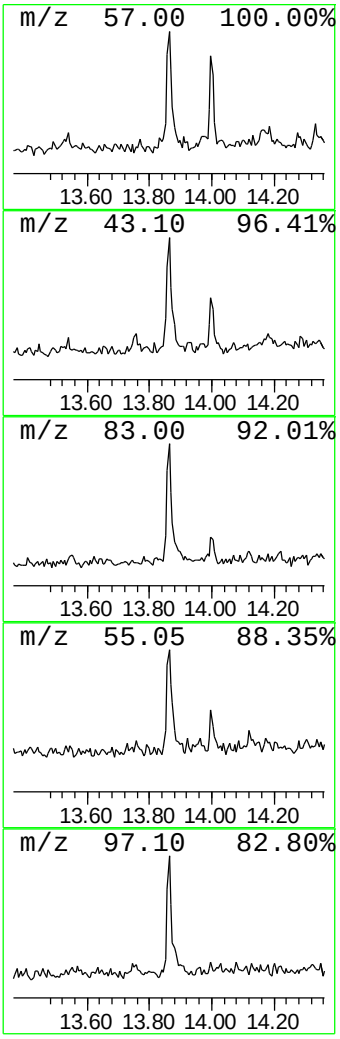
Peak Number 9 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.33 ng	117741	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
2	1-Heptacosanol	396	C27H56O	002004-39-9	87
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	81
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	74
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112017\
Data File : BF100742.D
Acq On : 20 Nov 2017 20:46
Operator : SJ/JU
Sample : I6521-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
2-Pentanone, 4-hy...	5.11	6.7	ng	184619	1	6.87	548208	20.0
unknown6.65	6.65	89.9	ng	2464000	1	6.87	548208	20.0
Hexadecane	9.83	2.0	ng	79646	3	9.90	782730	20.0
Tridecane	10.33	2.1	ng	84193	3	9.90	782730	20.0
Nonadecane	10.80	2.5	ng	93712	4	11.39	734079	20.0
n-Hexadecanoic acid	11.91	2.7	ng	100737	4	11.39	734079	20.0
unknown13.76	13.76	2.2	ng	59233	5	14.03	543957	20.0
n-Tetracosanol-1	13.86	4.3	ng	117741	5	14.03	543957	20.0