LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110558.D
Acq On : 7 Nov 2018 16:33
Operator : JU/SJ
Sample : J5839-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

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-BF102318.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	2.269	26	31	53	rVB	330144	510837	20.63%	1.652%
2	3.592	254	256	264	rBV	10345	25986	1.05%	0.084%
3	5.192	523	528	540	rBV	56364	78702	3.18%	0.255%
4	5.575	589	593	620	rVB	1757033	1907926	77.07%	6.170%
5	6.581	759	764	783	rBV	1946630	2121592	85.70%	6.861%
6	6.722	783	788	791	rBV	2262052	2031862	82.07%	6.571%
7	6.951	823	827	832	rBV	506307	432688	17.48%	1.399%
8	7.104	849	853	857	rBV	1732050	1582755	63.93%	5.119%
9	7.516	918	923	926	rBV	1297907	1260938	50.93%	4.078%
10	8.233	1041	1045	1060	rBV	582874	584228	23.60%	1.889%
11	9.310	1222	1228	1231	rBV	2502744	2475646	100.00%	8.006%
12	9.698	1290	1294	1300	rVB	344901	289851	11.71%	0.937%
13	9.992	1340	1344	1347	rBV	762660	639105	25.82%	2.067%
14	10.021	1347	1349	1356	rVB	51995	48659	1.97%	0.157%
15	10.198	1371	1379	1382	rBV2	29808	40506	1.64%	0.131%
16	10.545	1435	1438	1442	rVB	51124	48346	1.95%	0.156%
17	10.786	1475	1479	1490	rBV	1471485	1385797	55.98%	4.482%
18	11.486	1594	1598	1600	rBV	695686	614467	24.82%	1.987%
19	11.510	1600	1602	1607	rVV	196783	166660	6.73%	0.539%
20	11.563	1607	1611	1615	rVB	44838	47628	1.92%	0.154%
21	11.721	1636	1638	1642	rBV	36724	36537	1.48%	0.118%
22	11.986	1679	1683	1687	rBV	167003	211177	8.53%	0.683%
23	12.104	1700	1703	1706	rBV	28333	28424	1.15%	0.092%
24	12.651	1781	1796	1803	rBV	528947	1768878	71.45%	5.720%
25	12.704	1803	1805	1809	rVV	183231	181838	7.35%	0.588%
26	12.774	1813	1817	1829	rVB	227160	373338	15.08%	1.207%
27	12.915	1838	1841	1842	rBV	41879	32416	1.31%	0.105%
28	12.939	1842	1845	1850	rVB	103288	116917	4.72%	0.378%
29	13.068	1862	1867	1870	rBV	2245739	1995866	80.62%	6.454%
30	13.268	1897	1901	1905	rVB2	35943	45886	1.85%	0.148%
31	13.404	1920	1924	1933	rVB3	33289	76228	3.08%	0.247%
32	13.615	1956	1960	1963	rBV2	43677	46458	1.88%	0.150%
33	13.768	1975	1986	1994	rBV	590697	1705056	68.87%	5.514%
34	13.945	2012	2016	2027	rVB	209998	250904	10.13%	0.811%

LSC Area Percent Report

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Sample : J5839-03
Misc :
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Instrument : BNA_F
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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-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.133	2043	2048	2052	rBV	482896	530863	21.44%	1.717%
36	14.262	2064	2070	2072	rBV	235215	278457	11.25%	0.901%
37	14.498	2103	2110	2117	rBV	661893	1153547	46.60%	3.730%
38	14.562	2117	2121	2130	rVB	442806	471257	19.04%	1.524%
39	14.733	2148	2150	2153	rVB	34911	29925	1.21%	0.097%
40	14.880	2170	2175	2184	rBV2	639597	860999	34.78%	2.784%
41	15.162	2215	2223	2230	rBV	218714	588085	23.75%	1.902%
42	15.233	2230	2235	2247	rVB	554361	787876	31.83%	2.548%
43	15.627	2293	2302	2305	rBV2	459962	790960	31.95%	2.558%
44	15.662	2305	2308	2325	rVB2	442603	930504	37.59%	3.009%
45	15.945	2348	2356	2366	rVB2	108390	292107	11.80%	0.945%
46	16.086	2373	2380	2386	rVB	274527	450185	18.18%	1.456%
47	16.615	2463	2470	2486	rVB	142195	303766	12.27%	0.982%
48	16.862	2505	2512	2522	rVB4	32262	116919	4.72%	0.378%
49	17.239	2571	2576	2584	rVB2	58891	126764	5.12%	0.410%
50	17.933	2688	2694	2697	rBV6	18390	45814	1.85%	0.148%

Sum of corrected areas: 30922130

LSC Report - Integrated Chromatogram

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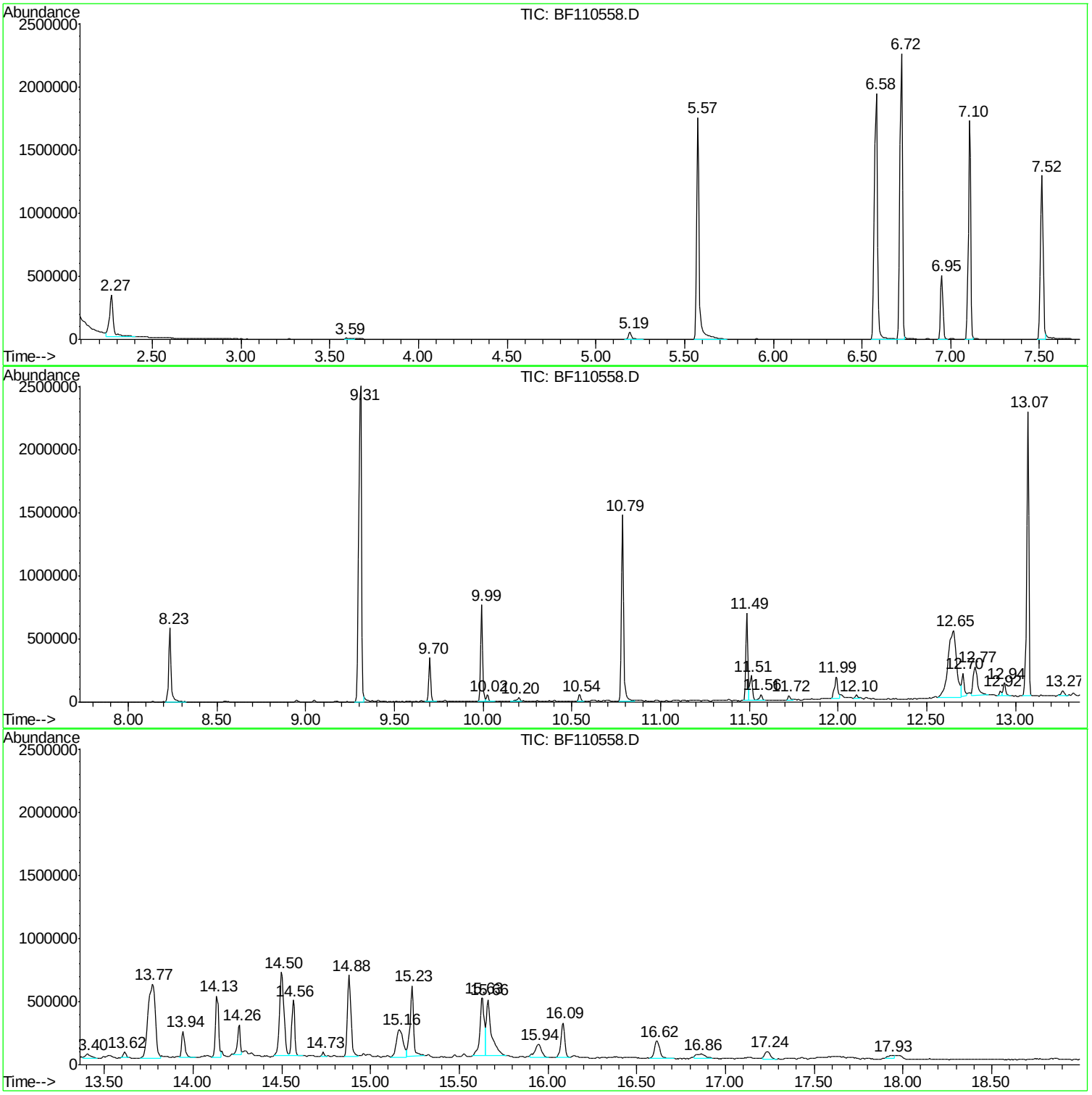
Operator : JU/SJ
Sample : J5839-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110558.D
Acq On : 7 Nov 2018 16:33
Operator : JU/SJ
Sample : J5839-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

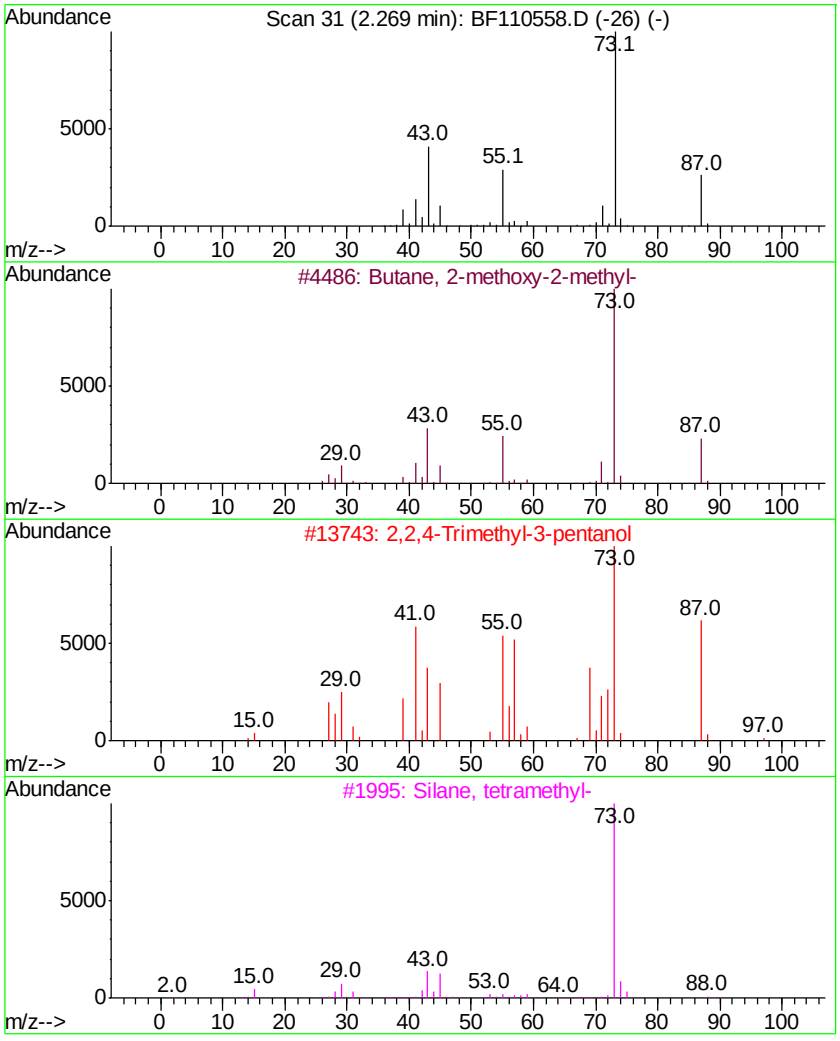
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

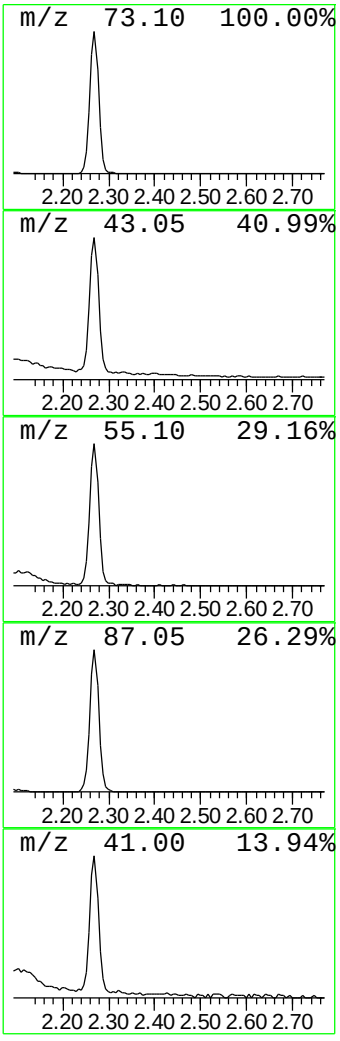
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	23.61 ng	510837	1,4-Dichlorobenzene-d4	6.95

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	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10





Library Search Compound Report

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Operator : JU/SJ
Sample : J5839-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

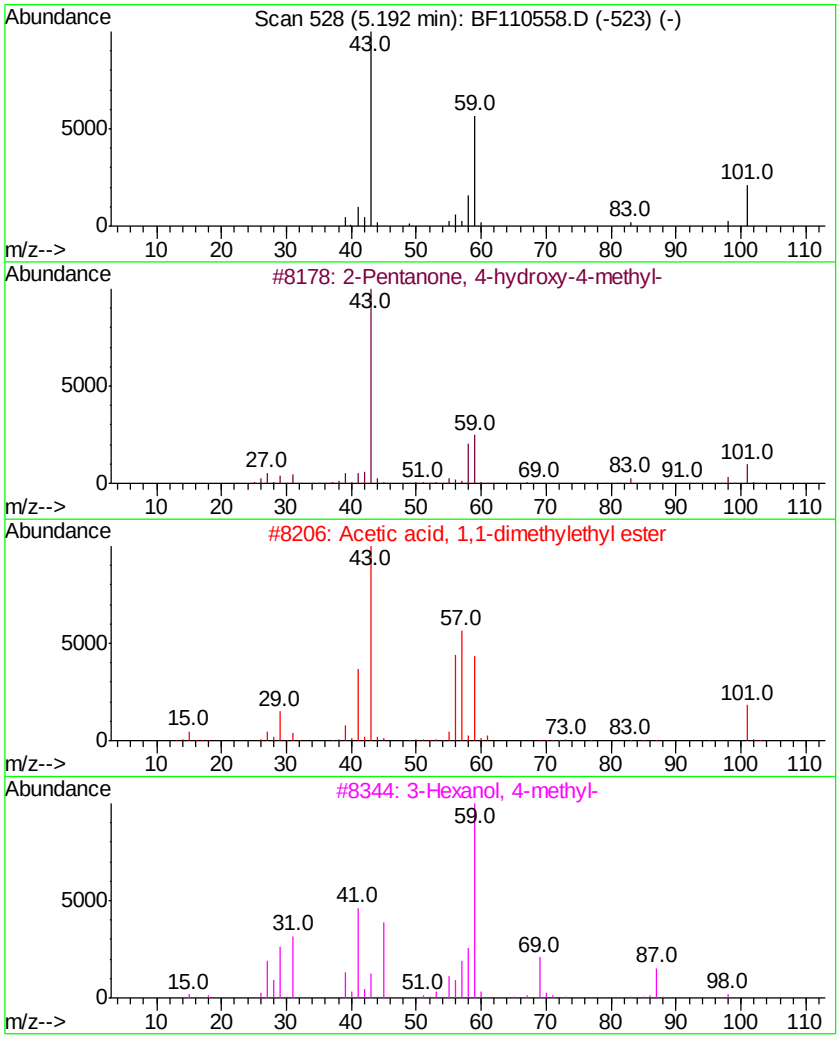
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

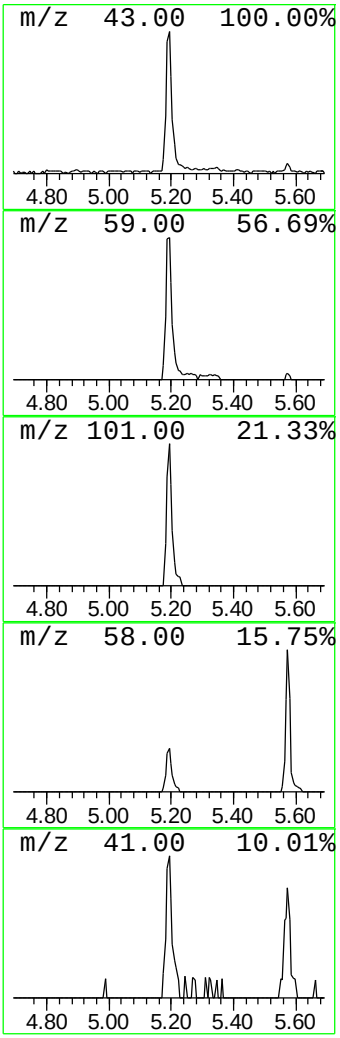
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.64 ng	78702	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Library Search Compound Report

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Acq On : 7 Nov 2018 16:33
Operator : JU/SJ
Sample : J5839-03
Misc :
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Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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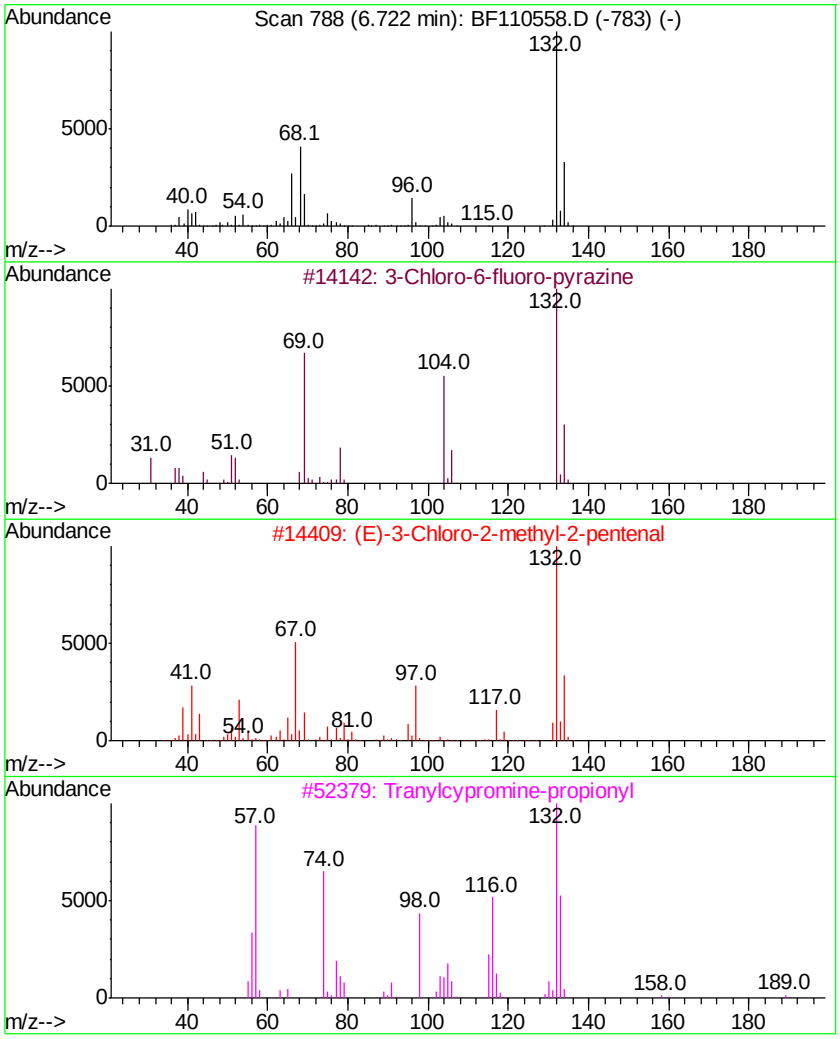
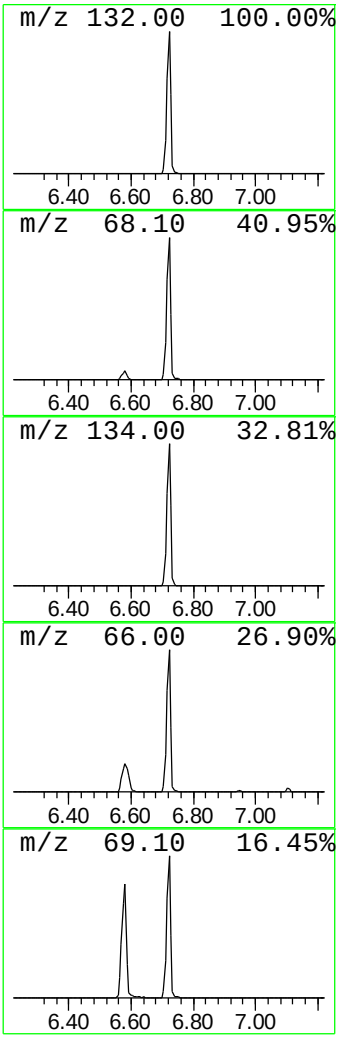
****

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	93.92 ng	2031860	1,4-Dichlorobenzene-d4	6.95

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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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
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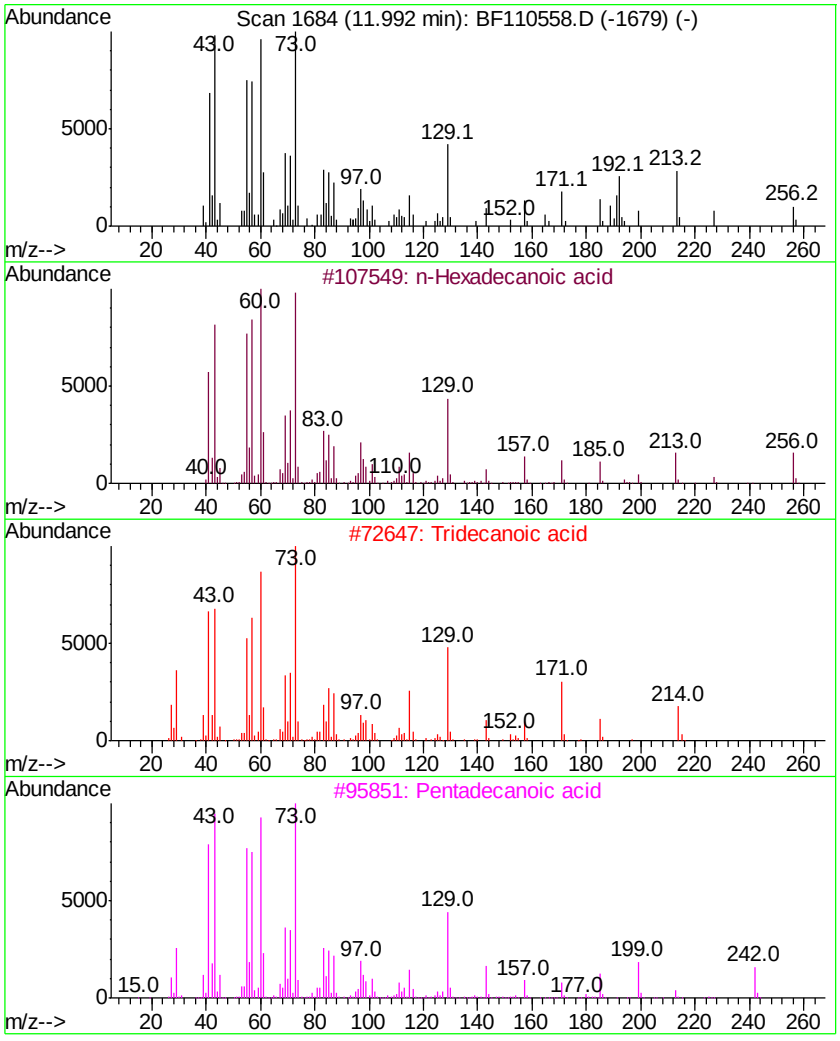
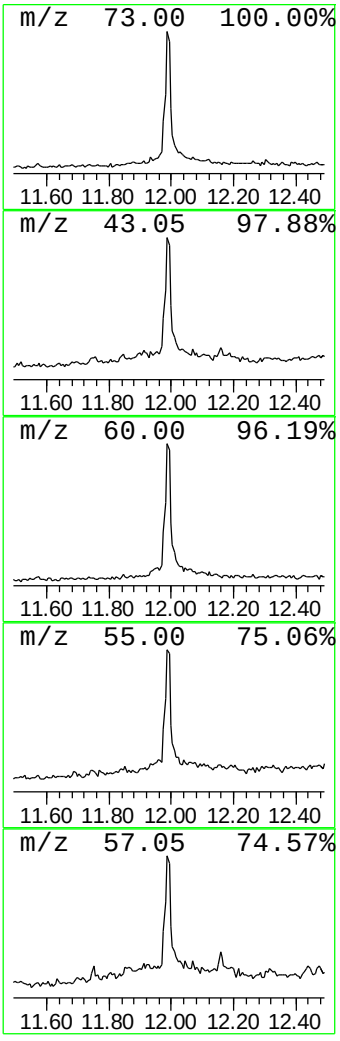
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	6.87 ng	211177	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





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Instrument : BNA_F
ClientSampleId : SB-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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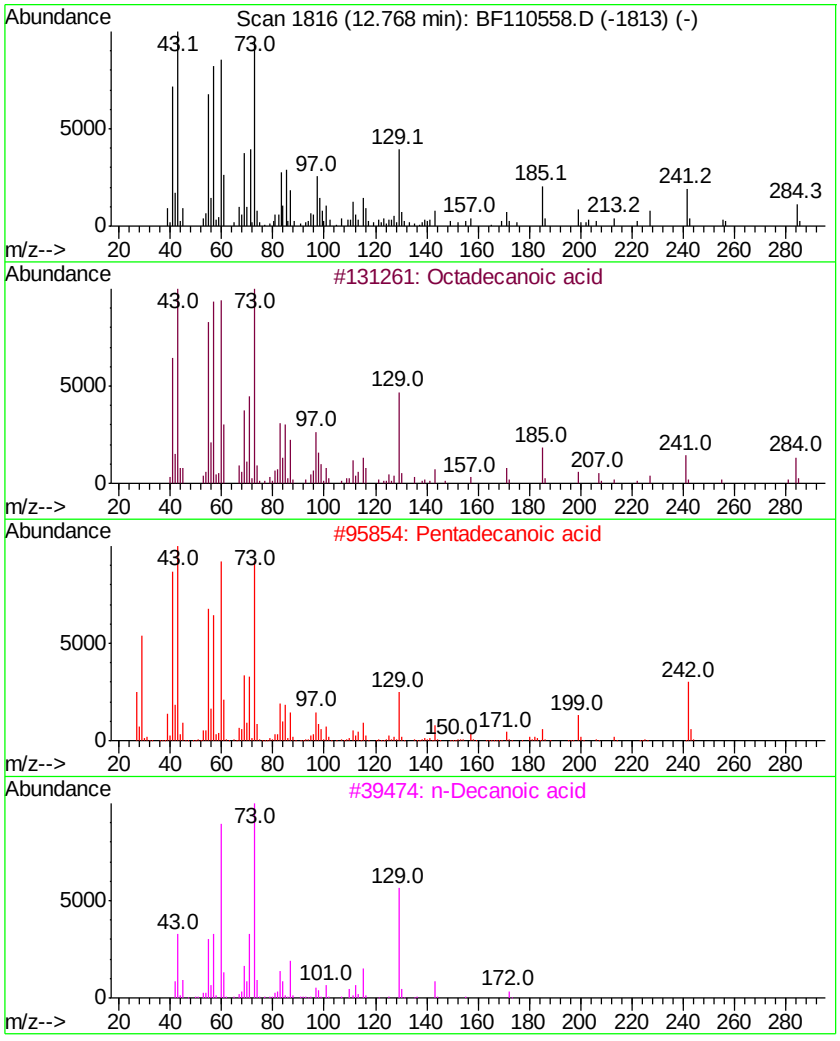
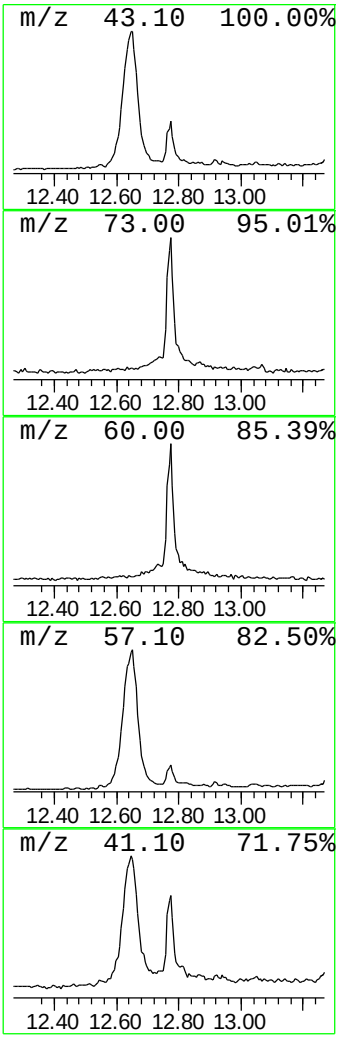
****

Peak Number 7 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	12.15 ng	373338	Phenanthrene-d10	11.49

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	n-Decanoic acid	172	C10H20O2	000334-48-5	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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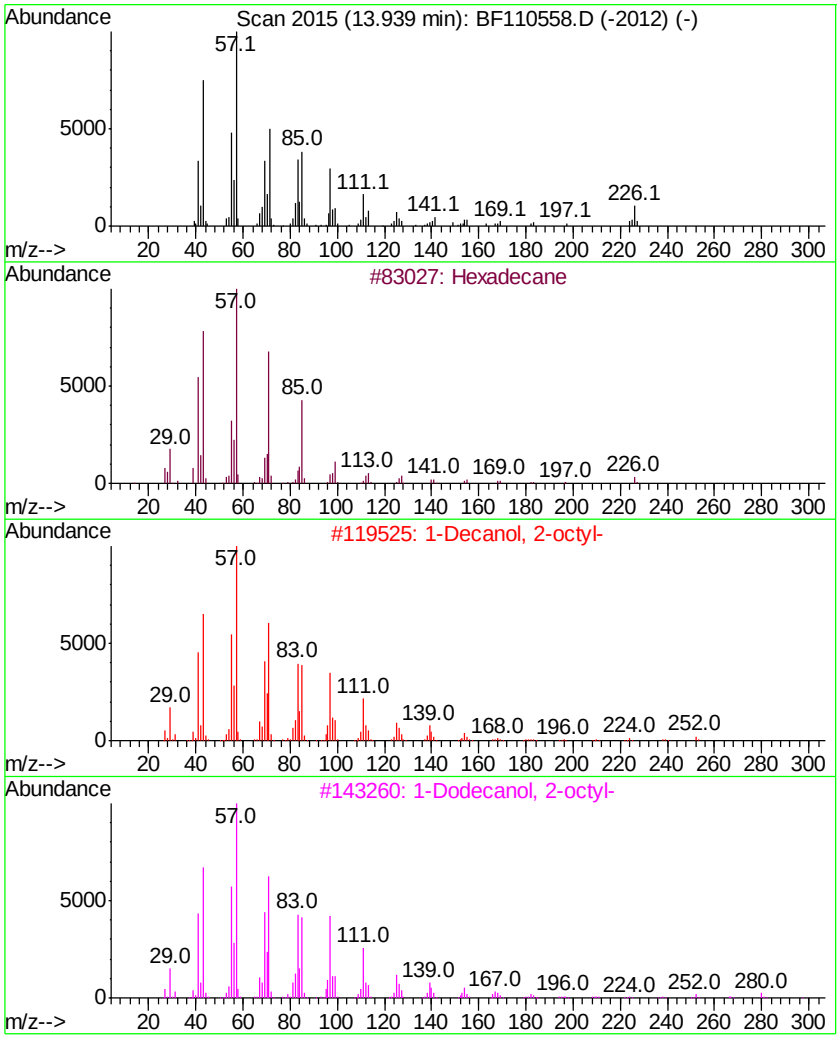
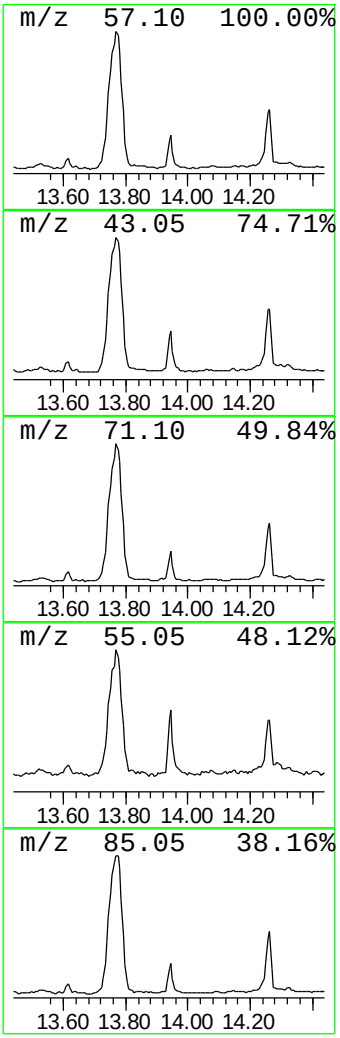
Peak Number 10 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	9.45 ng	250904	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	91
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
5	Cetene	224	C16H32	000629-73-2	86





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Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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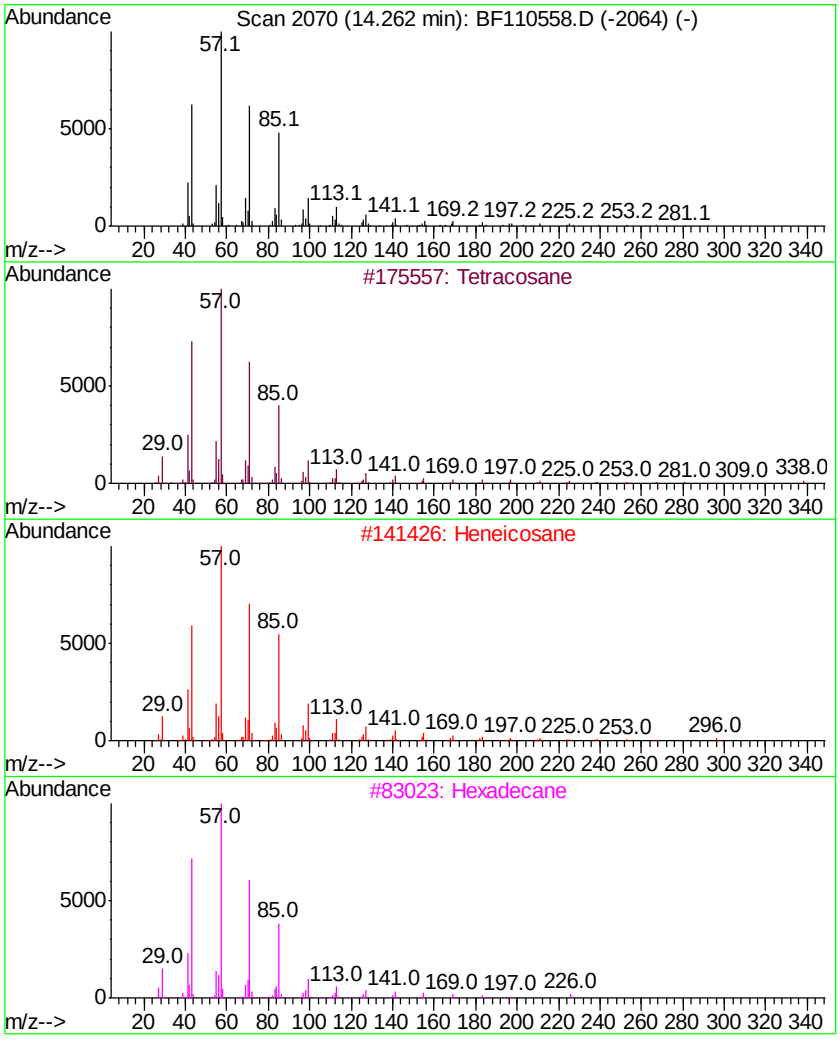
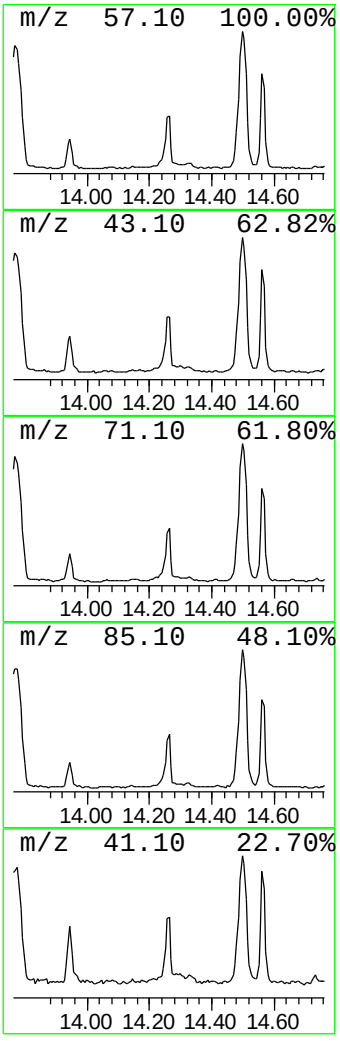
Peak Number 11 Tetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	10.49 ng	278457	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Octadecane	254	C18H38	000593-45-3	87





Library Search Compound Report

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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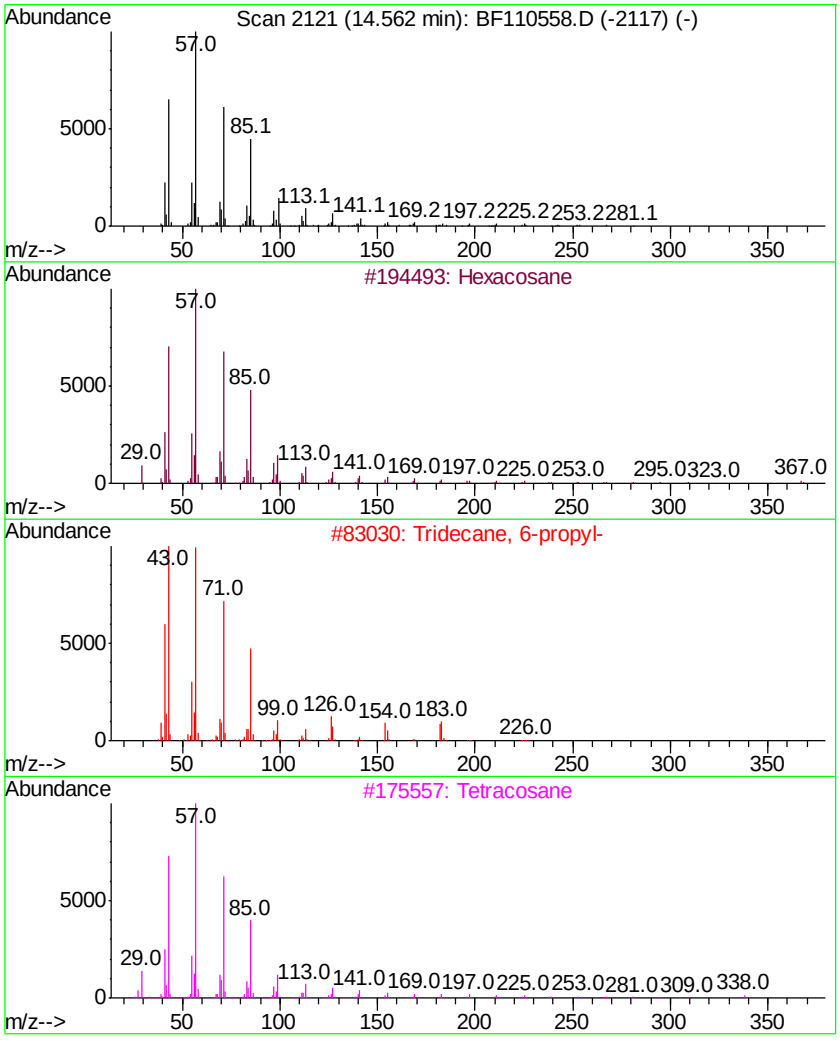
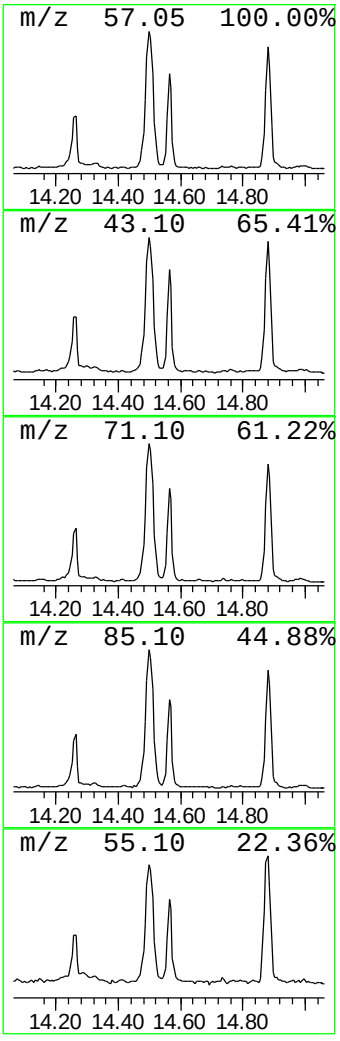
Peak Number 13 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	17.75 ng	471257	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Tridecane, 6-propyl-	226	C16H34	055045-10-8	93
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Octacosane	394	C28H58	000630-02-4	91





Library Search Compound Report

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Data File : BF110558.D
Acq On : 7 Nov 2018 16:33
Operator : JU/SJ
Sample : J5839-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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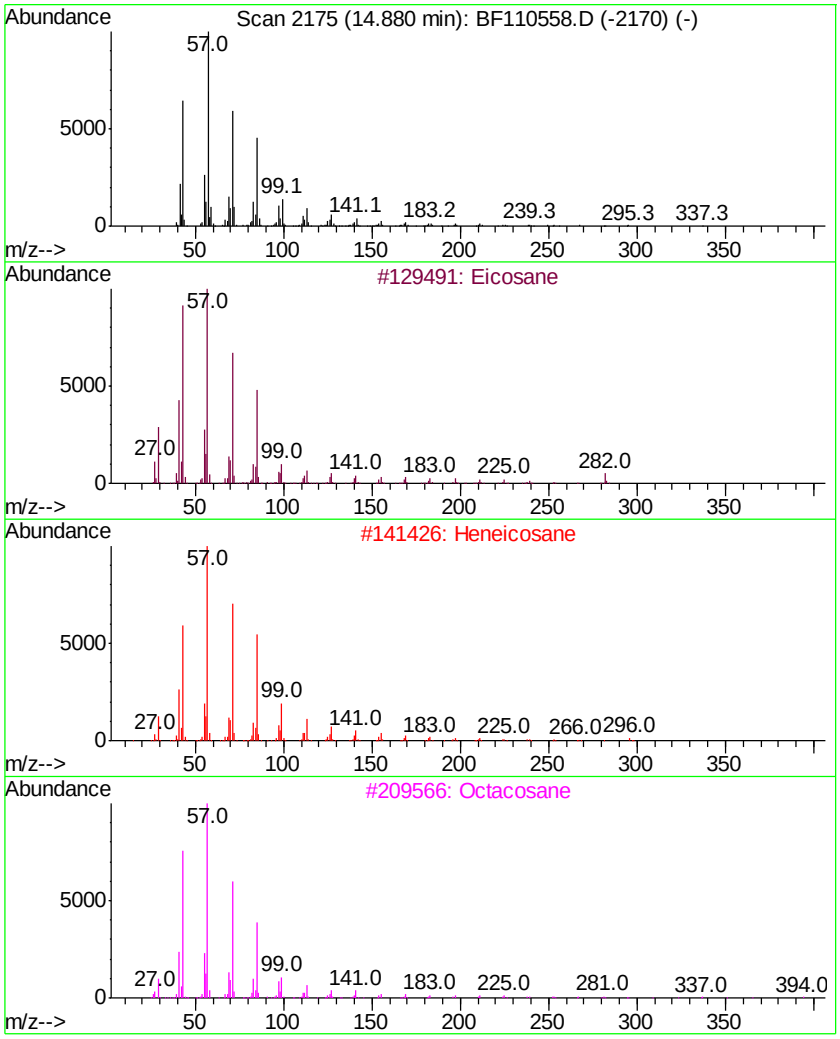
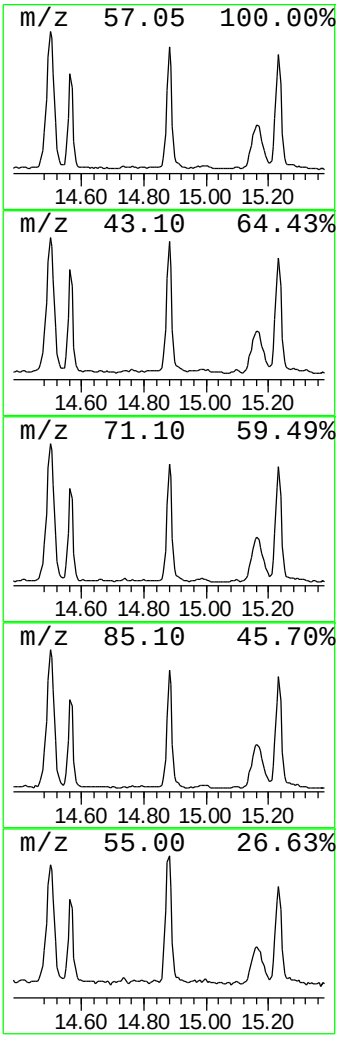
Peak Number 14 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	32.44 ng	860999	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Octadecane	254	C18H38	000593-45-3	83





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Acq On : 7 Nov 2018 16:33
Operator : JU/SJ
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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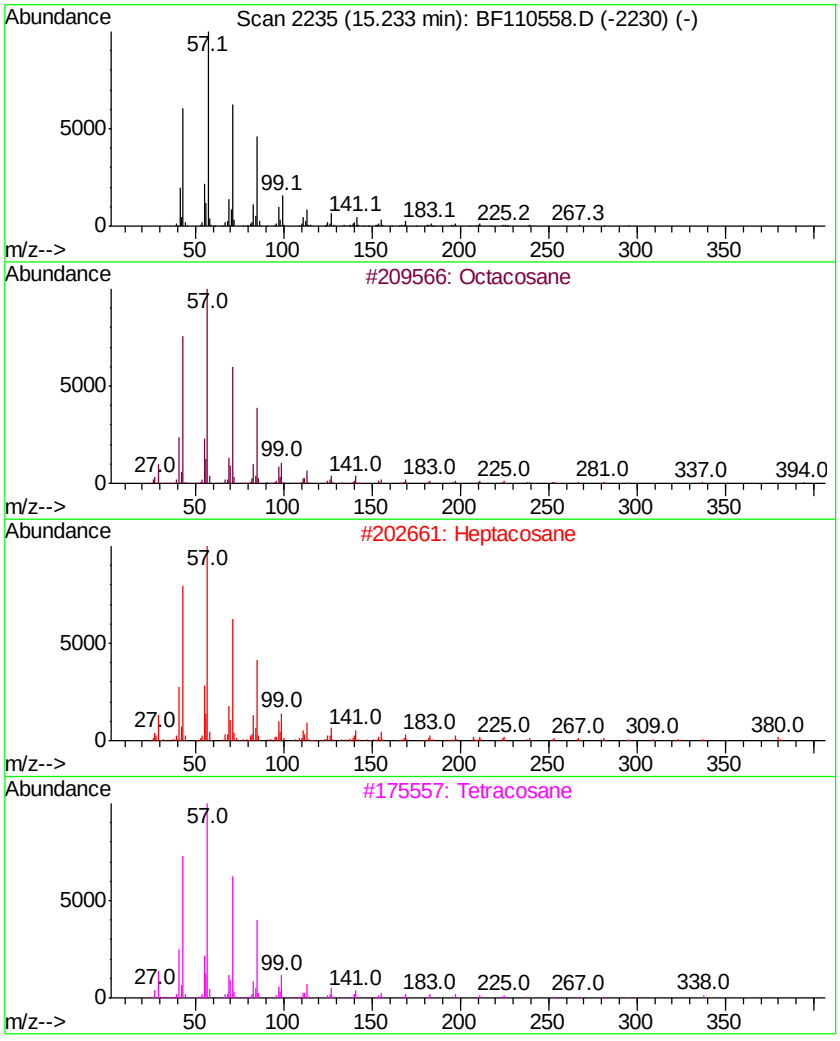
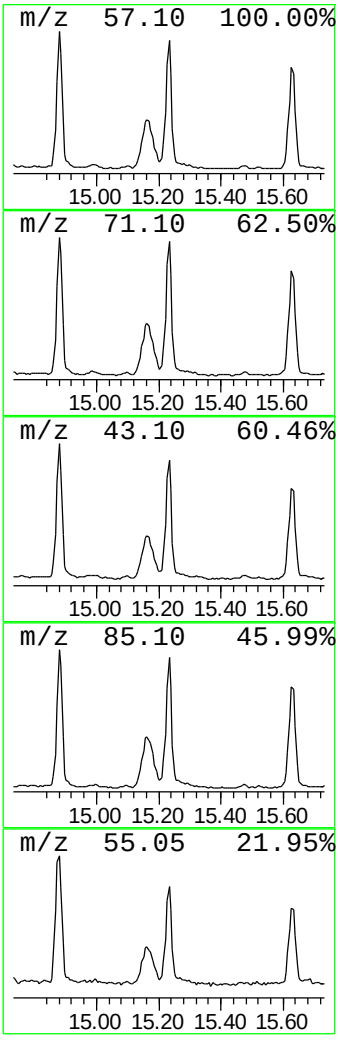
Peak Number 16 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	16.93 ng	787876	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Data File : BF110558.D
Acq On : 7 Nov 2018 16:33
Operator : JU/SJ
Sample : J5839-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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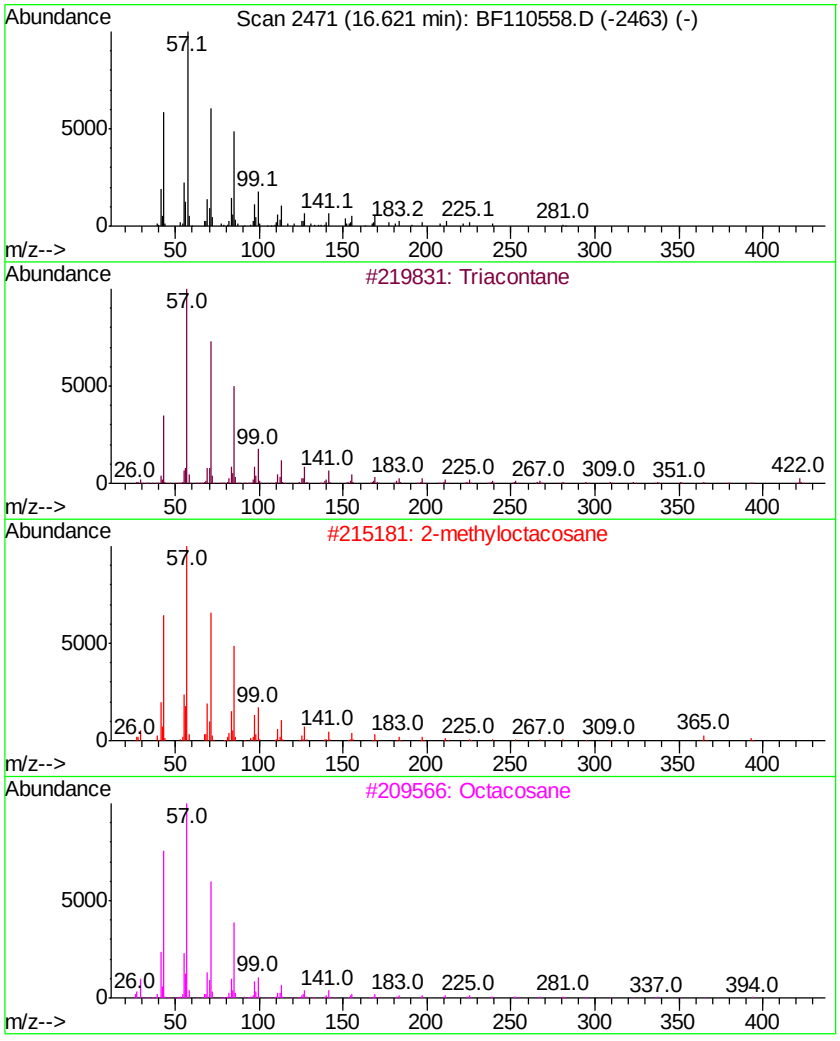
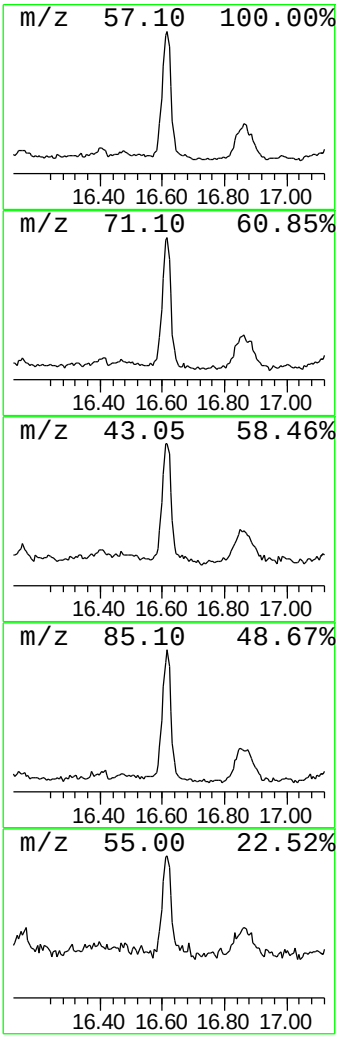
Peak Number 19 Triacontane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	6.53 ng	303766	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Docosane	310	C22H46	000629-97-0	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110558.D
Acq On : 7 Nov 2018 16:33
Operator : JU/SJ
Sample : J5839-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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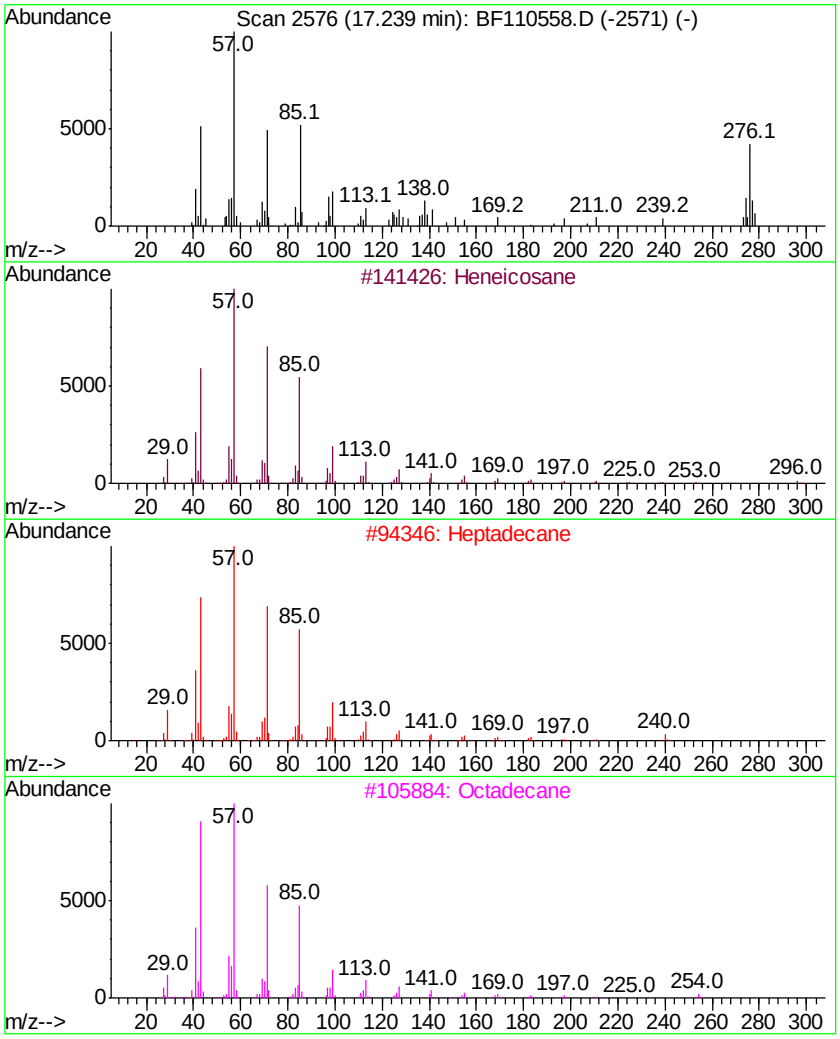
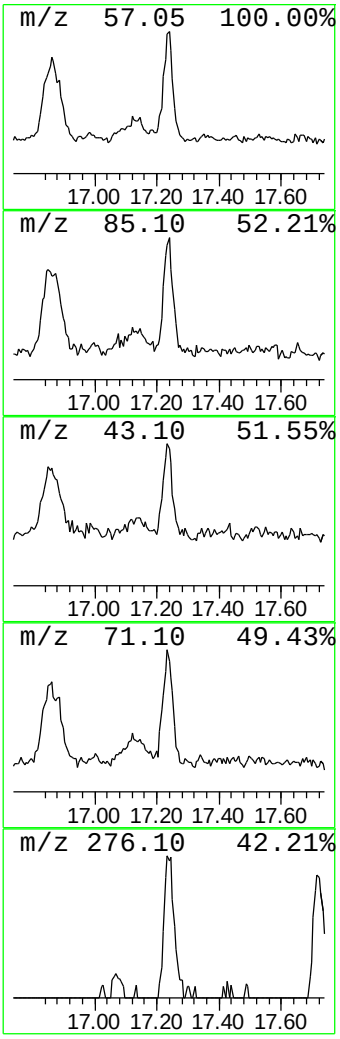
Peak Number 20 Heneicosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.24	2.72 ng	126764	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	45
2	Heptadecane	240	C17H36	000629-78-7	43
3	Octadecane	254	C18H38	000593-45-3	38
4	Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	38
5	Nonacosane	408	C29H60	000630-03-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110718\
Data File : BF110558.D
Acq On : 7 Nov 2018 16:33
Operator : JU/SJ
Sample : J5839-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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
Butane, 2-methoxy...	2.27	23.6	ng	510837	1	6.95	432688	20.0
2-Pentanone, 4-hy...	5.19	3.6	ng	78702	1	6.95	432688	20.0
unknown6.72	6.72	93.9	ng	2031860	1	6.95	432688	20.0
n-Hexadecanoic acid	11.99	6.9	ng	211177	4	11.49	614467	20.0
Octadecanoic acid	12.77	12.2	ng	373338	4	11.49	614467	20.0
Hexadecane	13.94	9.4	ng	250904	5	14.13	530863	20.0
Tetracosane	14.26	10.5	ng	278457	5	14.13	530863	20.0
Hexacosane	14.56	17.8	ng	471257	5	14.13	530863	20.0
Eicosane	14.88	32.4	ng	860999	5	14.13	530863	20.0
Octacosane	15.23	16.9	ng	787876	6	15.66	930504	20.0
Triacontane	16.62	6.5	ng	303766	6	15.66	930504	20.0
Heneicosane	17.24	2.7	ng	126764	6	15.66	930504	20.0