LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110211.D
Acq On : 26 Oct 2018 15:56
Operator : JU/SJ
Sample : J5621-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-SB-01A

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	2.322	33	40	47	rVB	321640	426513	13.67%	1.522%
2	4.604	424	428	432	rBV	27877	32377	1.04%	0.116%
3	5.210	527	531	543	rVB	212595	270075	8.66%	0.964%
4	5.469	571	575	578	rBV	104526	95703	3.07%	0.341%
5	5.592	589	596	600	rBV2	2683187	3094240	99.17%	11.041%
6	5.828	632	636	640	rBV	210461	183277	5.87%	0.654%
7	5.875	642	644	647	rVB	51973	38992	1.25%	0.139%
8	6.522	750	754	757	rVB	89348	74604	2.39%	0.266%
9	6.592	760	766	772	rBV2	2568174	3120175	100.00%	11.133%
10	6.739	786	791	794	rBV	3047263	2756565	88.35%	9.836%
11	6.792	797	800	804	rBV	91567	78750	2.52%	0.281%
12	6.969	826	830	833	rBV	919118	743927	23.84%	2.654%
13	7.122	850	856	860	rBV	2300896	2150170	68.91%	7.672%
14	7.528	921	925	933	rBV	1704272	1770452	56.74%	6.317%
15	8.251	1044	1048	1051	rBV	1099319	925249	29.65%	3.301%
16	8.963	1166	1169	1176	rBV	58355	59520	1.91%	0.212%
17	9.063	1183	1186	1189	rBV	47279	41224	1.32%	0.147%
18	9.327	1226	1231	1234	rBV	2795634	2673664	85.69%	9.540%
19	9.663	1285	1288	1291	rBV	32190	32318	1.04%	0.115%
20	9.716	1294	1297	1305	rVB	400391	348674	11.17%	1.244%
21	9.922	1327	1332	1337	rBV	34386	32260	1.03%	0.115%
22	10.010	1344	1347	1351	rBV	1080260	888870	28.49%	3.172%
23	10.210	1375	1381	1385	rVB2	26793	35967	1.15%	0.128%
24	10.422	1410	1417	1421	rBV2	39576	48844	1.57%	0.174%
25	10.798	1477	1481	1488	rBV	1389827	1370482	43.92%	4.890%
26	10.910	1495	1500	1507	rVB3	48019	80781	2.59%	0.288%
27	11.504	1597	1601	1603	rBV	926031	772604	24.76%	2.757%
28	11.527	1603	1605	1609	rVB	109363	90078	2.89%	0.321%
29	12.010	1683	1687	1689	rBV2	126123	120731	3.87%	0.431%
30	12.033	1689	1691	1695	rVB2	50078	47856	1.53%	0.171%
31	12.298	1732	1736	1739	rBV	26949	31785	1.02%	0.113%
32	12.721	1804	1808	1812	rBV	164519	154886	4.96%	0.553%
33	12.951	1841	1847	1853	rVB	168264	202833	6.50%	0.724%
34	13.086	1866	1870	1873	rBV	2106204	1771726	56.78%	6.322%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SA-SB-01A

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	13.157	1880	1882	1888	rBV5	18989	34364	1.10%	0.123%
36	13.298	1904	1906	1909	rVB	40507	33164	1.06%	0.118%
37	13.639	1961	1964	1968	rBV2	53870	66433	2.13%	0.237%
38	13.968	2017	2020	2033	rVB2	246222	323845	10.38%	1.156%
39	14.151	2046	2051	2054	rBV	737468	760310	24.37%	2.713%
40	14.174	2054	2055	2058	rVB	93916	53213	1.71%	0.190%
41	14.286	2071	2074	2080	rBV	106918	107849	3.46%	0.385%
42	14.592	2123	2126	2136	rVB2	168039	235590	7.55%	0.841%
43	14.915	2177	2181	2184	rVB	182121	205765	6.59%	0.734%
44	15.221	2230	2233	2236	rBV	62341	86286	2.77%	0.308%
45	15.268	2238	2241	2245	rVB	222971	257389	8.25%	0.918%
46	15.609	2296	2299	2303	rVV	41294	53639	1.72%	0.191%
47	15.674	2305	2310	2325	rVB2	497243	791831	25.38%	2.825%
48	16.133	2383	2388	2394	rVB	173778	271512	8.70%	0.969%
49	16.674	2475	2480	2488	rVB2	88741	178735	5.73%	0.638%

Sum of corrected areas: 28026097

LSC Report - Integrated Chromatogram

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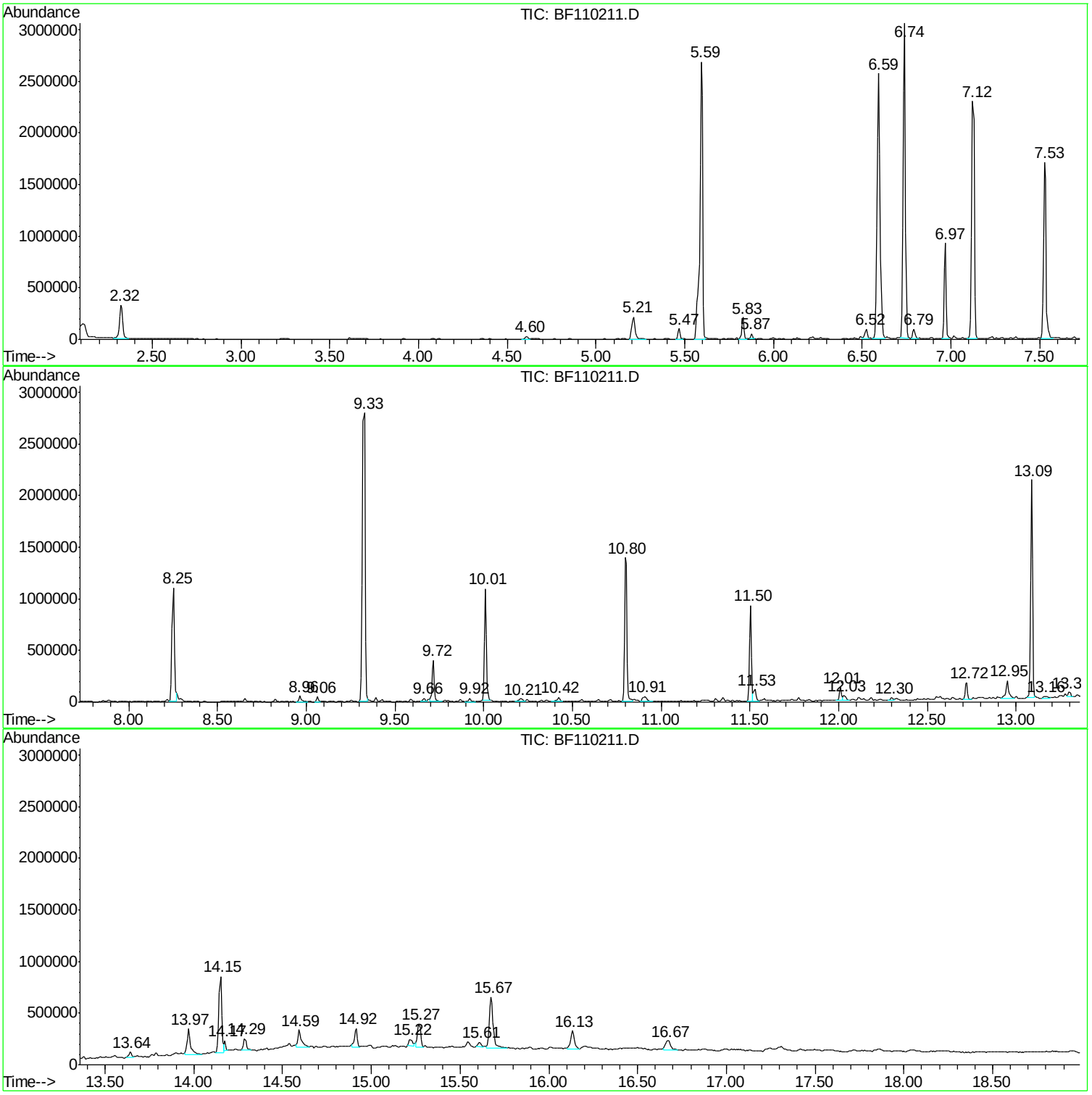
Sample : J5621-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-SB-01A

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



Library Search Compound Report

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Acq On : 26 Oct 2018 15:56
Operator : JU/SJ
Sample : J5621-05
Misc :
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Instrument : BNA_F
ClientSampleId : SA-SB-01A

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

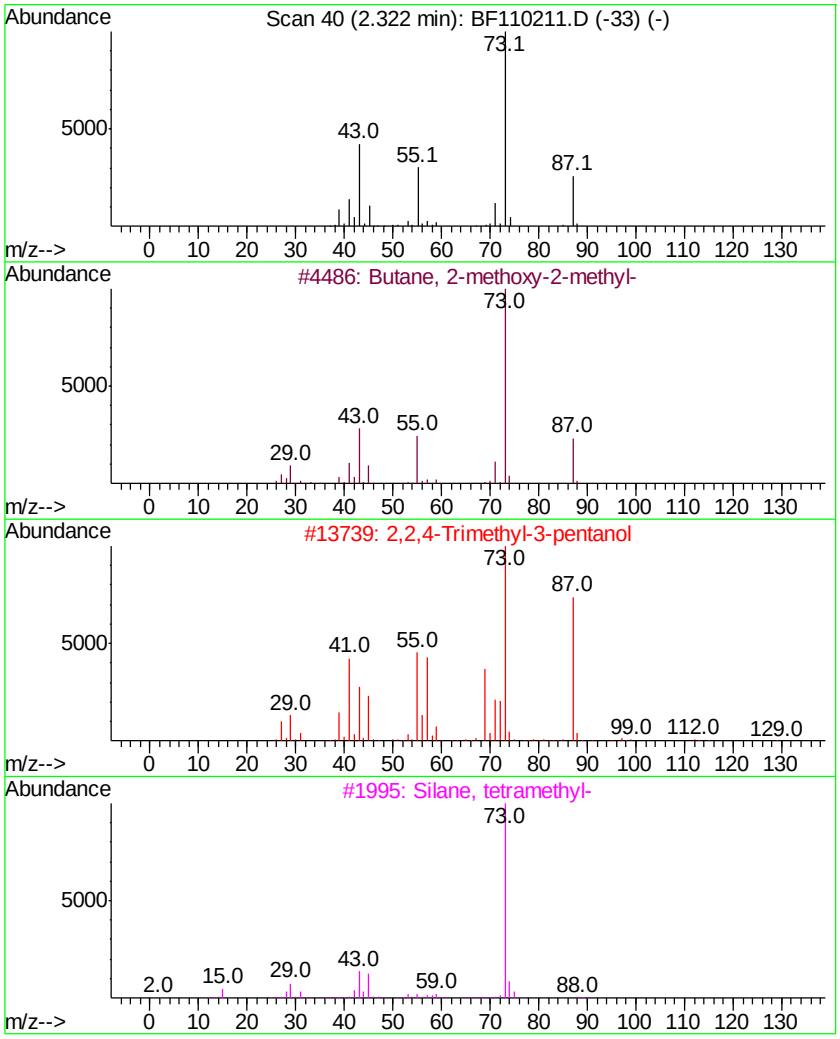
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

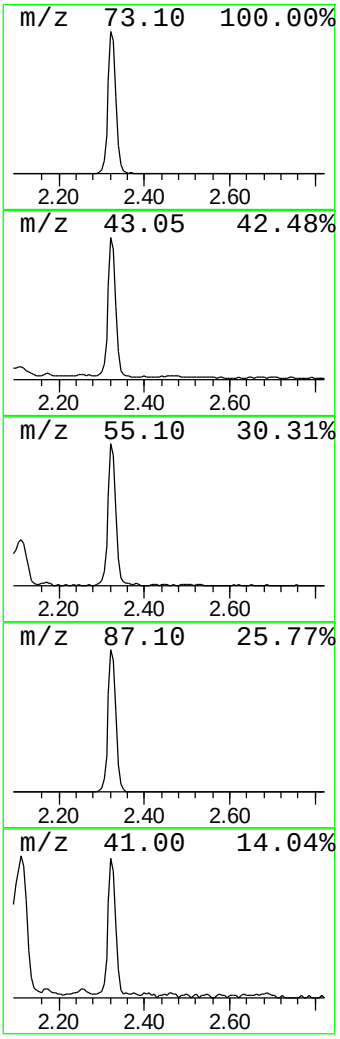
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	11.47 ng	426513	1,4-Dichlorobenzene-d4	6.97

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	38
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-SB-01A

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

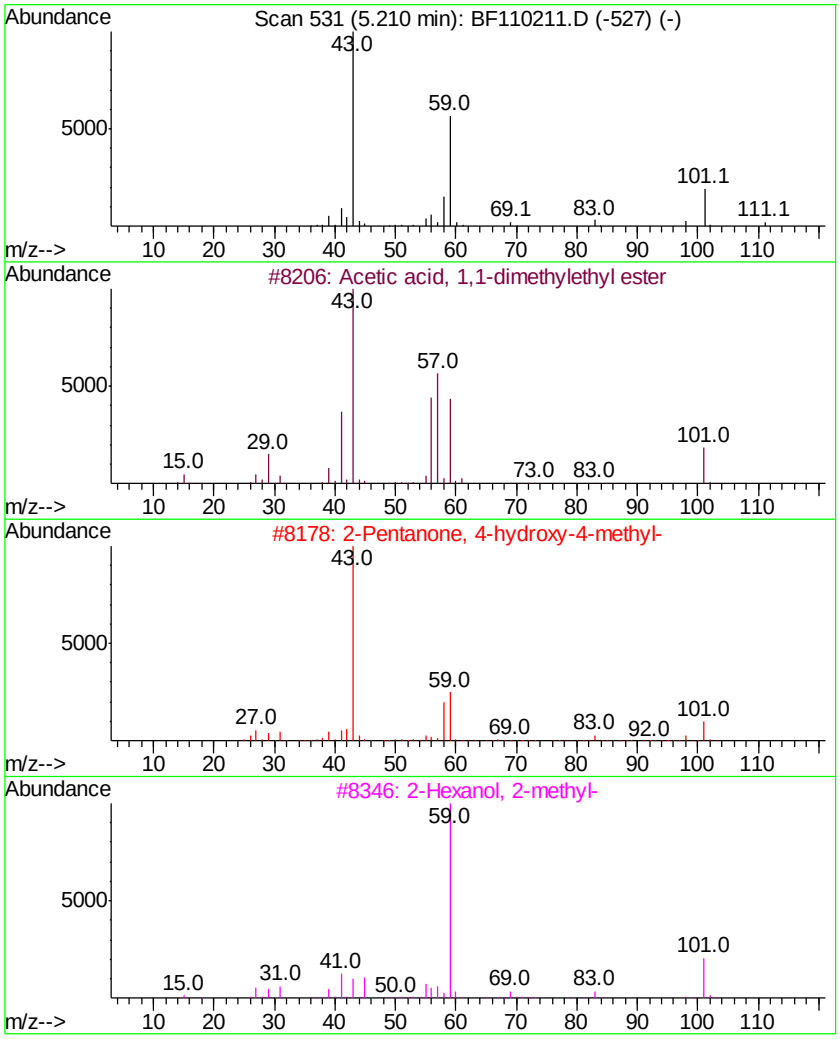
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

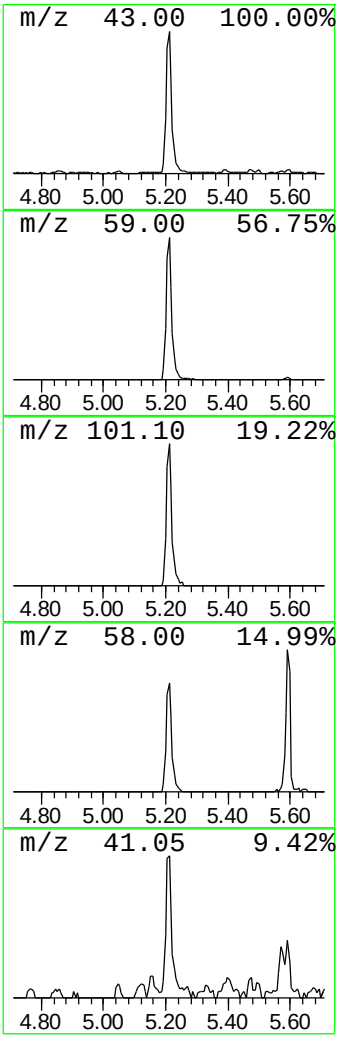
****

Peak Number 2 Acetic acid, 1,1-dimethylet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	7.26 ng	270075	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	10





Library Search Compound Report

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Acq On : 26 Oct 2018 15:56
Operator : JU/SJ
Sample : J5621-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-SB-01A

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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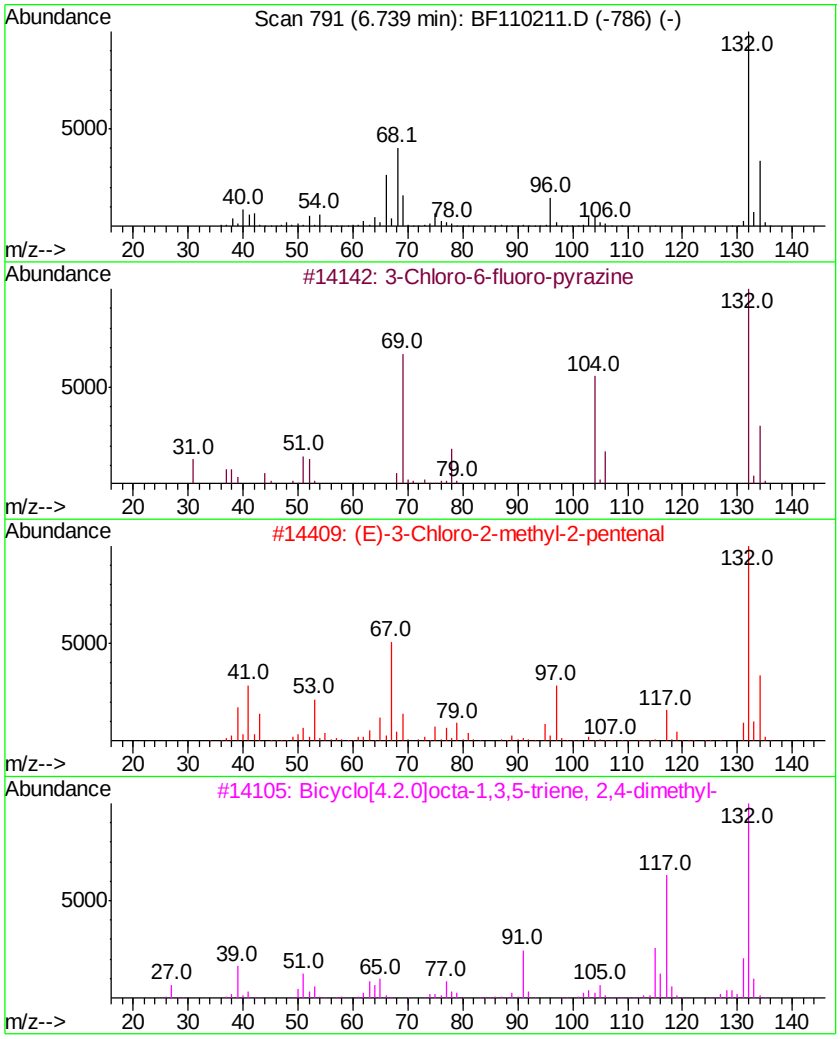
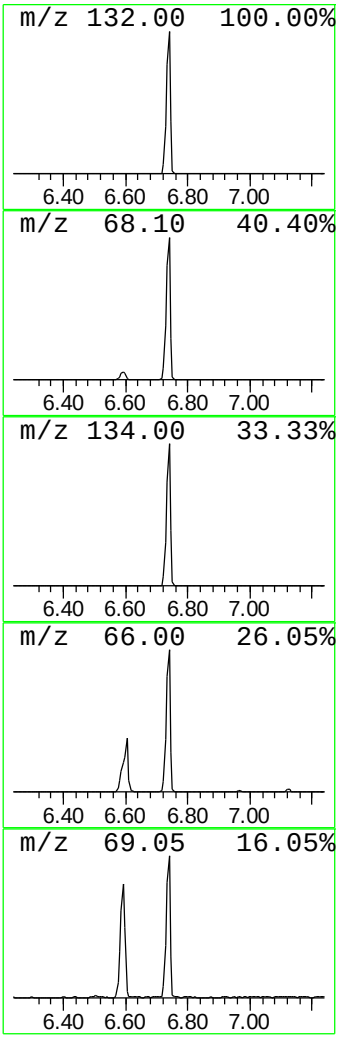
Peak Number 6 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	74.11 ng	2756570	1,4-Dichlorobenzene-d4	6.97

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Misc :
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Instrument : BNA_F
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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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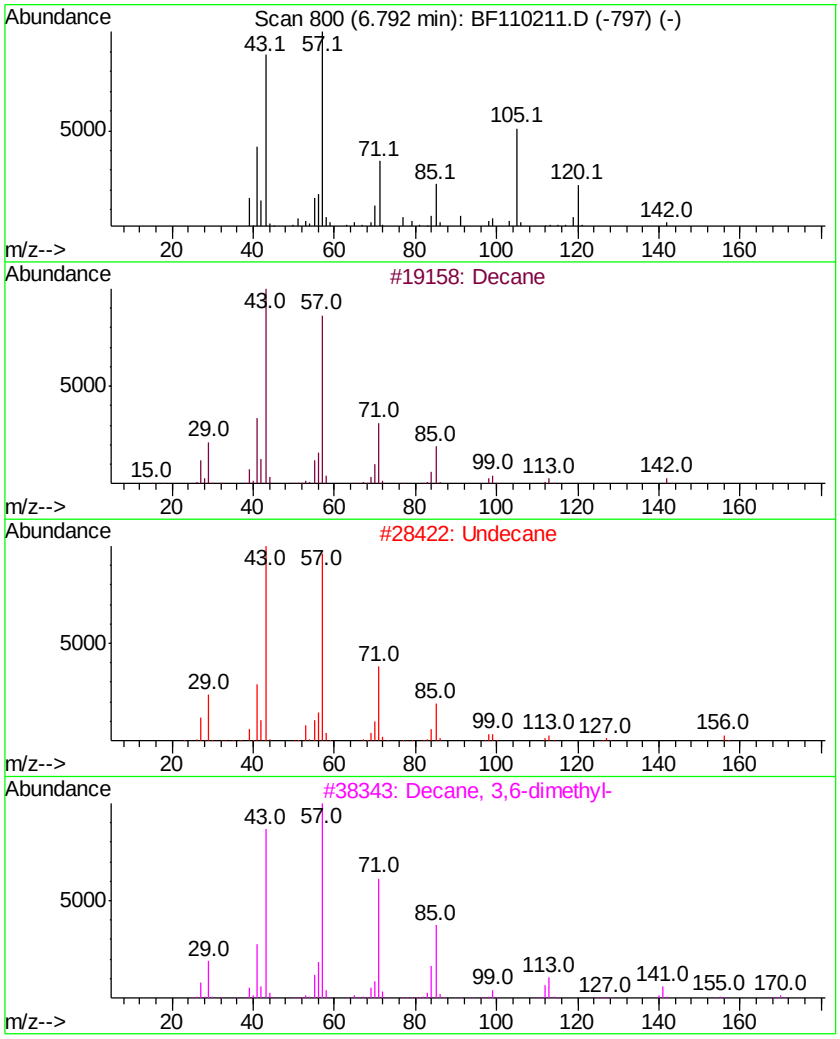
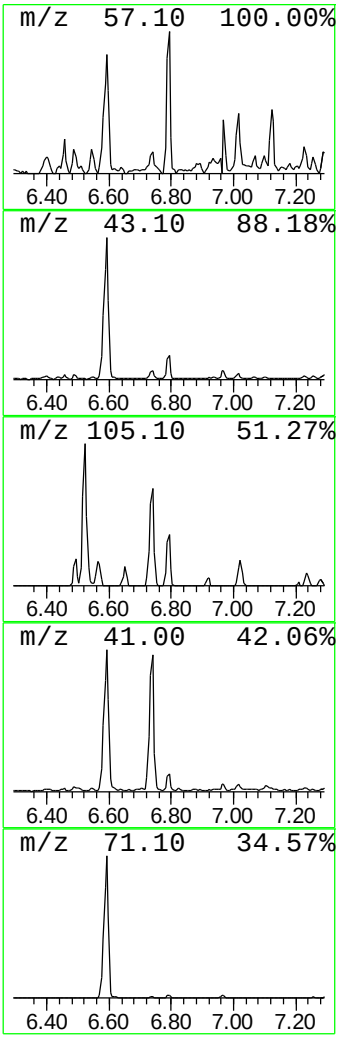
****

Peak Number 7 Decane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	2.12 ng	78750	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	90
2	Undecane	156	C11H24	001120-21-4	46
3	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	43
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	38
5	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	35





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Instrument : BNA_F
ClientSampleId : SA-SB-01A

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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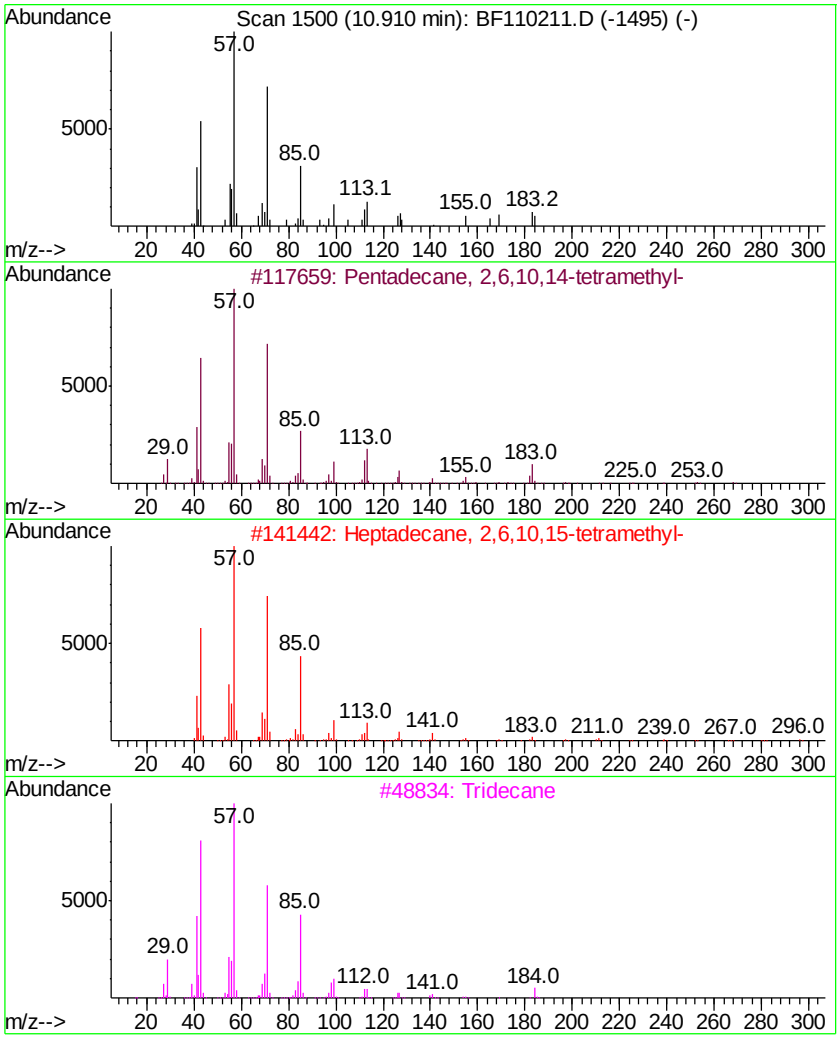
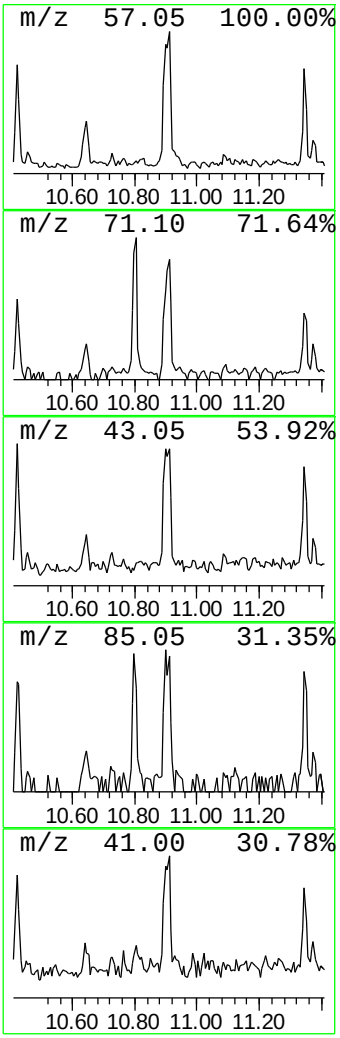
****

Peak Number 9 Pentadecane, 2,6,10,14-tetr... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	2.09 ng	80781	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	90
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
3	Tridecane	184	C13H28	000629-50-5	64
4	Tridecane, 3-methyl-	198	C14H30	006418-41-3	59
5	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	53





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ClientSampleId : SA-SB-01A

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TIC Library : C:\DATABASE\NIST11.L
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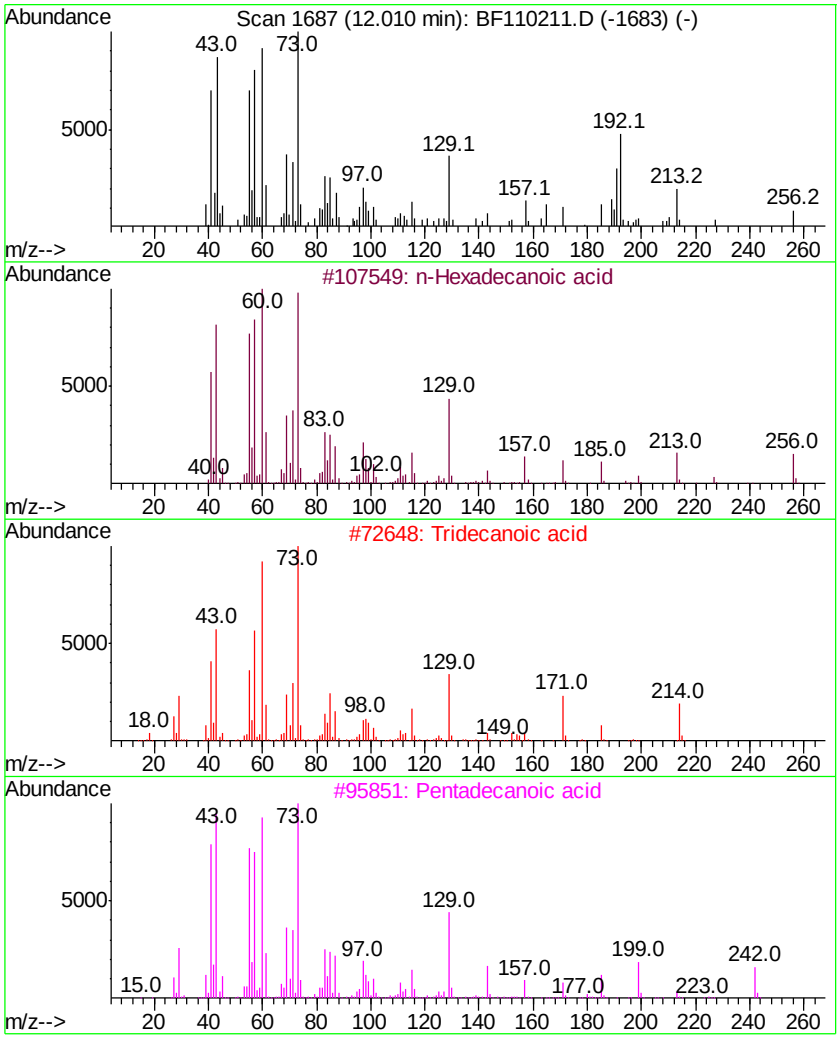
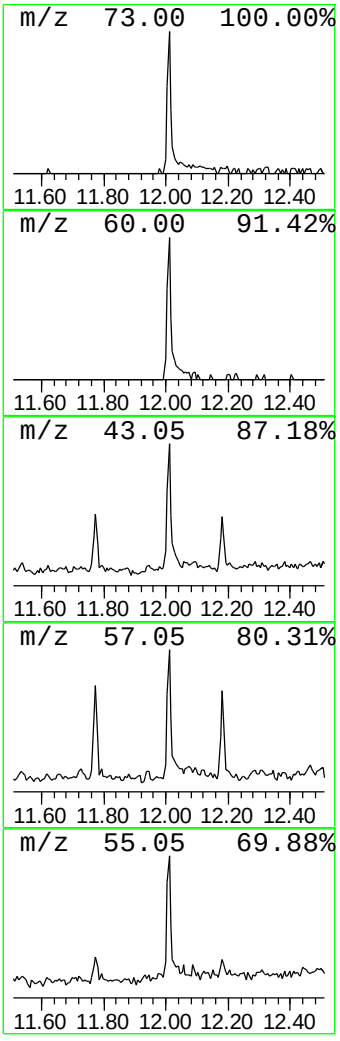
Peak Number 10 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	3.13 ng	120731	Phenanthrene-d10	11.50

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	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





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Misc :
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Instrument : BNA_F
ClientSampleId : SA-SB-01A

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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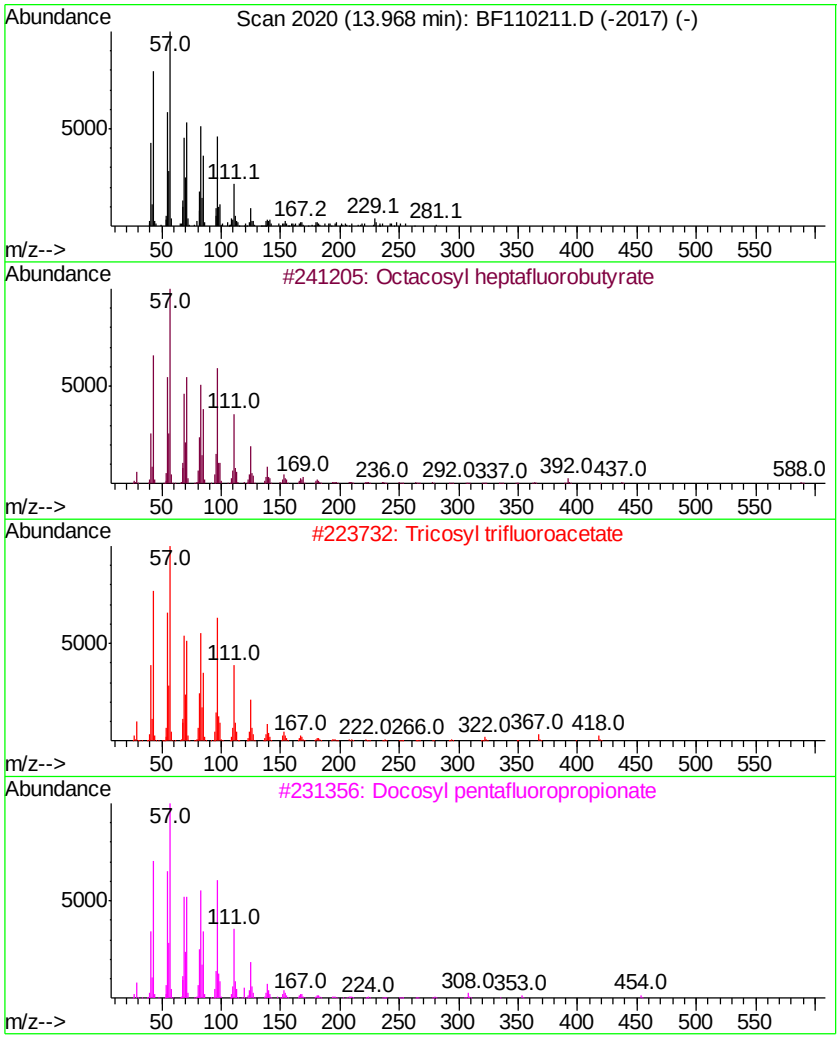
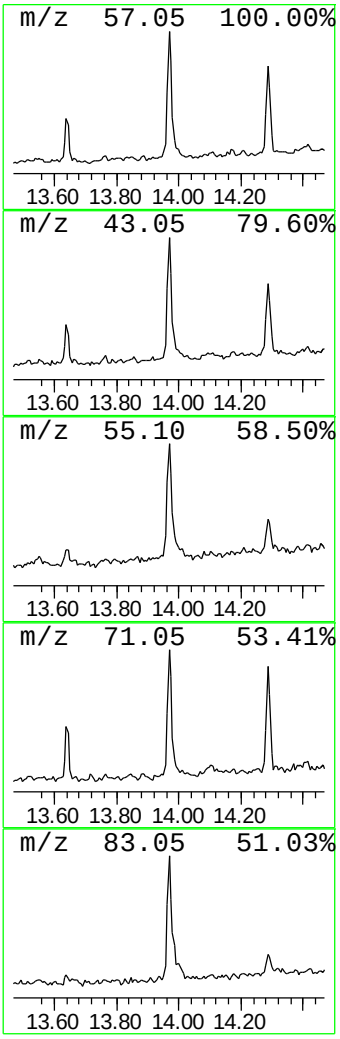
Peak Number 11 Octacosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	8.52 ng	323845	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
5	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91





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Data File : BF110211.D
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Sample : J5621-05
Misc :
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Instrument : BNA_F
ClientSampleId : SA-SB-01A

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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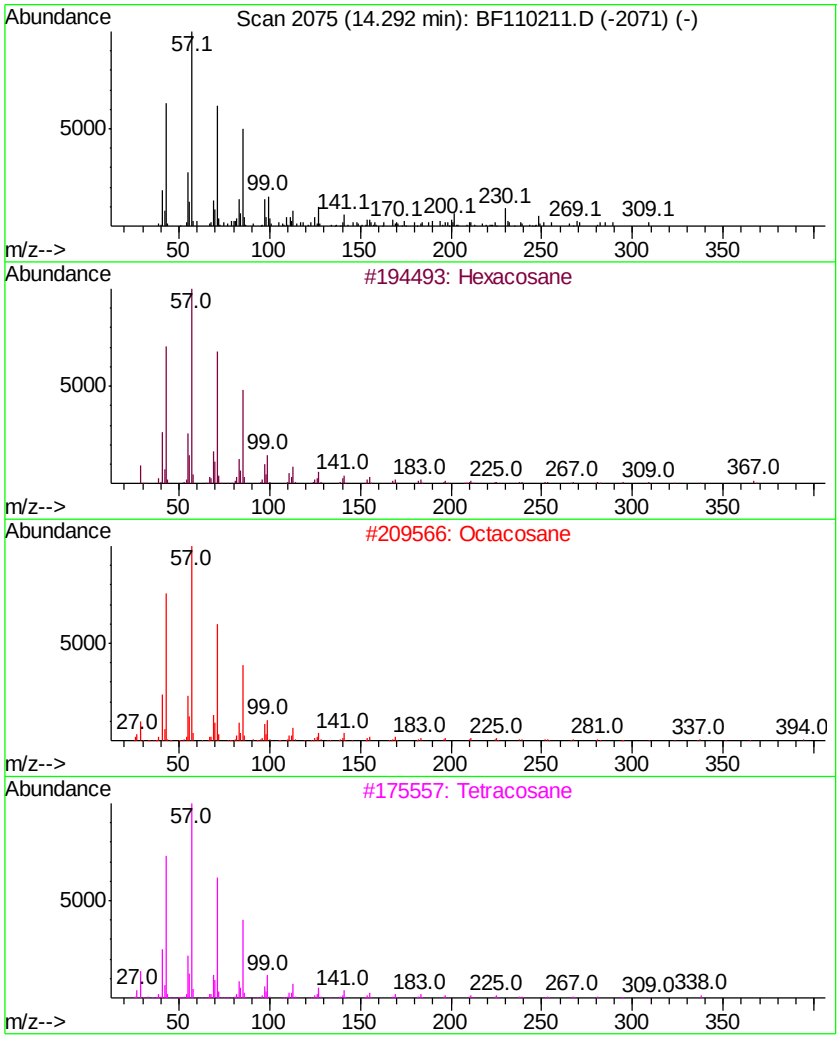
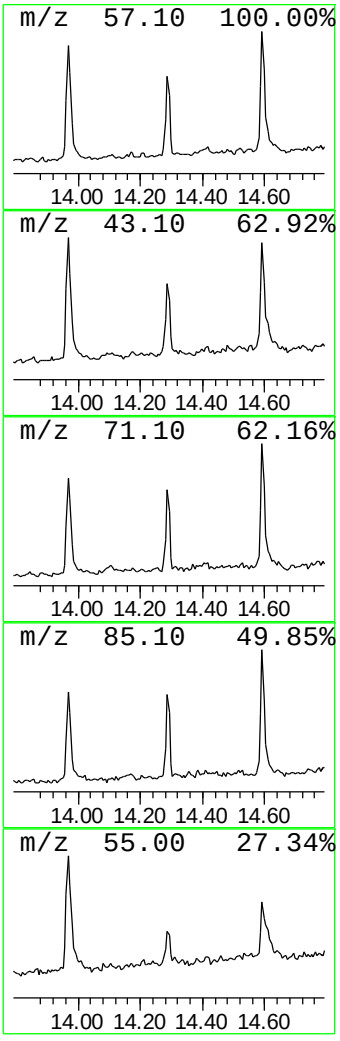
Peak Number 12 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.84 ng	107849	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Tetracosane	338	C24H50	000646-31-1	83
4	2-methyloctacosane	408	C29H60	1000376-72-8	83
5	Heneicosane	296	C21H44	000629-94-7	83





Library Search Compound Report

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Data File : BF110211.D
Acq On : 26 Oct 2018 15:56
Operator : JU/SJ
Sample : J5621-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-SB-01A

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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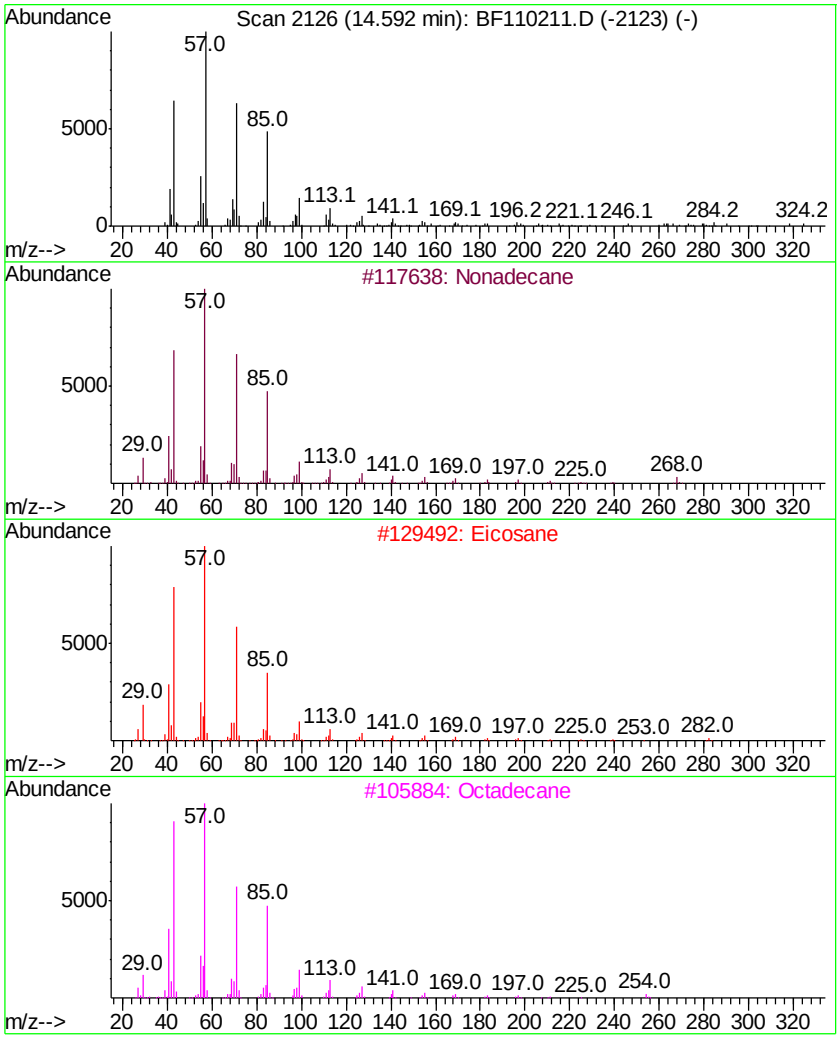
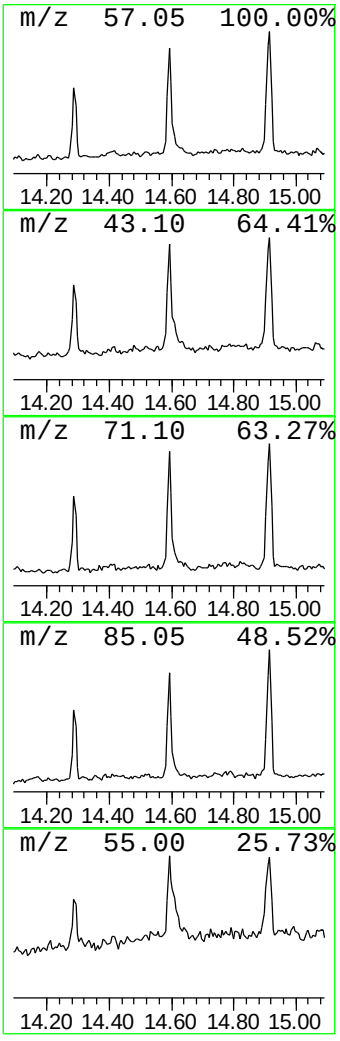
Peak Number 13 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	6.20 ng	235590	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	87
2	Eicosane	282	C20H42	000112-95-8	87
3	Octadecane	254	C18H38	000593-45-3	87
4	1-Iodoundecane	282	C11H23I	004282-44-4	87
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	87





Library Search Compound Report

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Acq On : 26 Oct 2018 15:56
Operator : JU/SJ
Sample : J5621-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-SB-01A

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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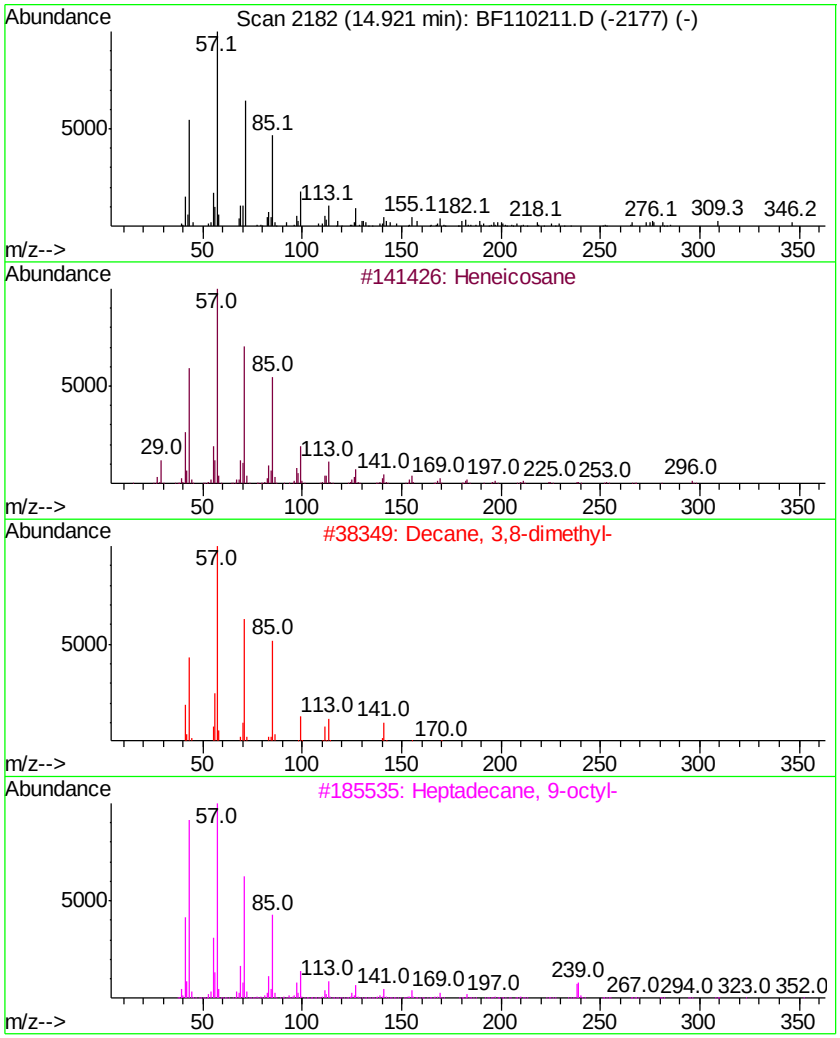
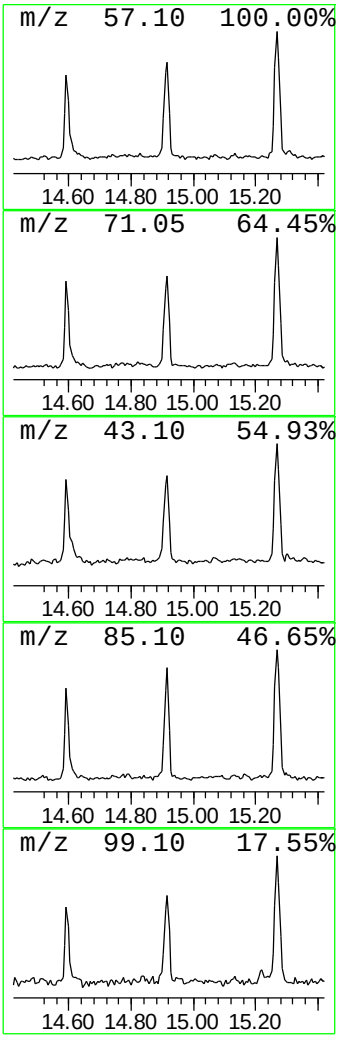
Peak Number 14 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	5.20 ng	205765	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





Library Search Compound Report

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Data File : BF110211.D
Acq On : 26 Oct 2018 15:56
Operator : JU/SJ
Sample : J5621-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-SB-01A

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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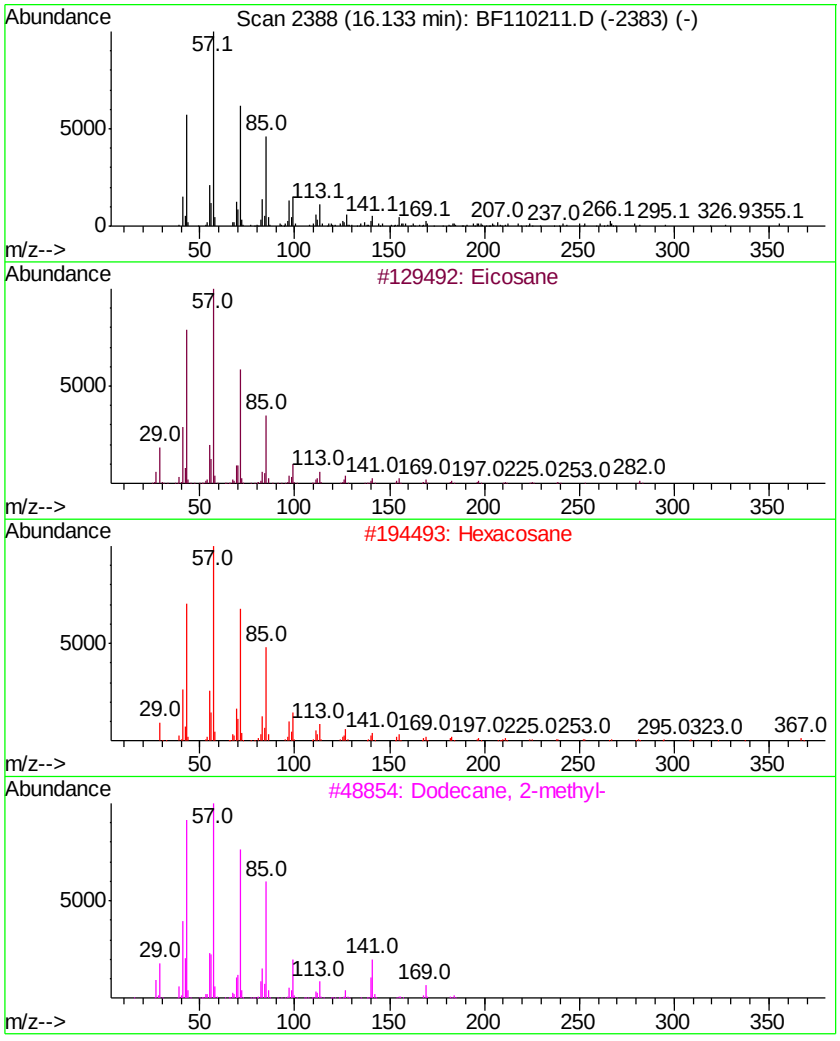
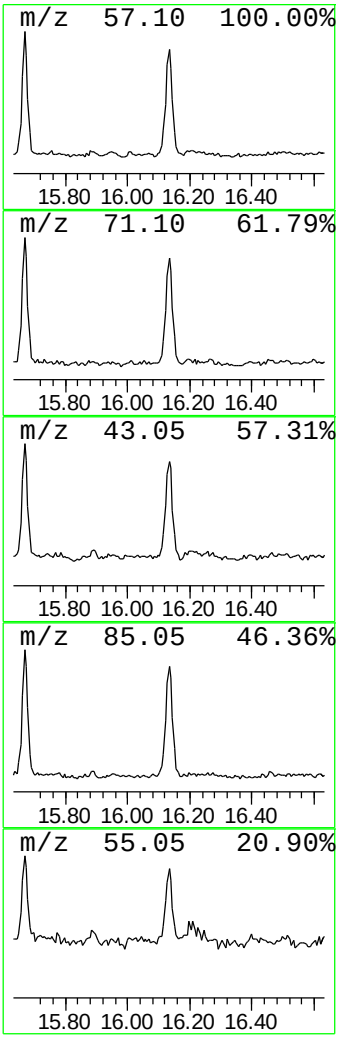
Peak Number 15 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	6.86 ng	271512	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hexacosane	366	C26H54	000630-01-3	90
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87





Library Search Compound Report

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Data File : BF110211.D
Acq On : 26 Oct 2018 15:56
Operator : JU/SJ
Sample : J5621-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-SB-01A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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TIC Integration Parameters: LSCINT.P

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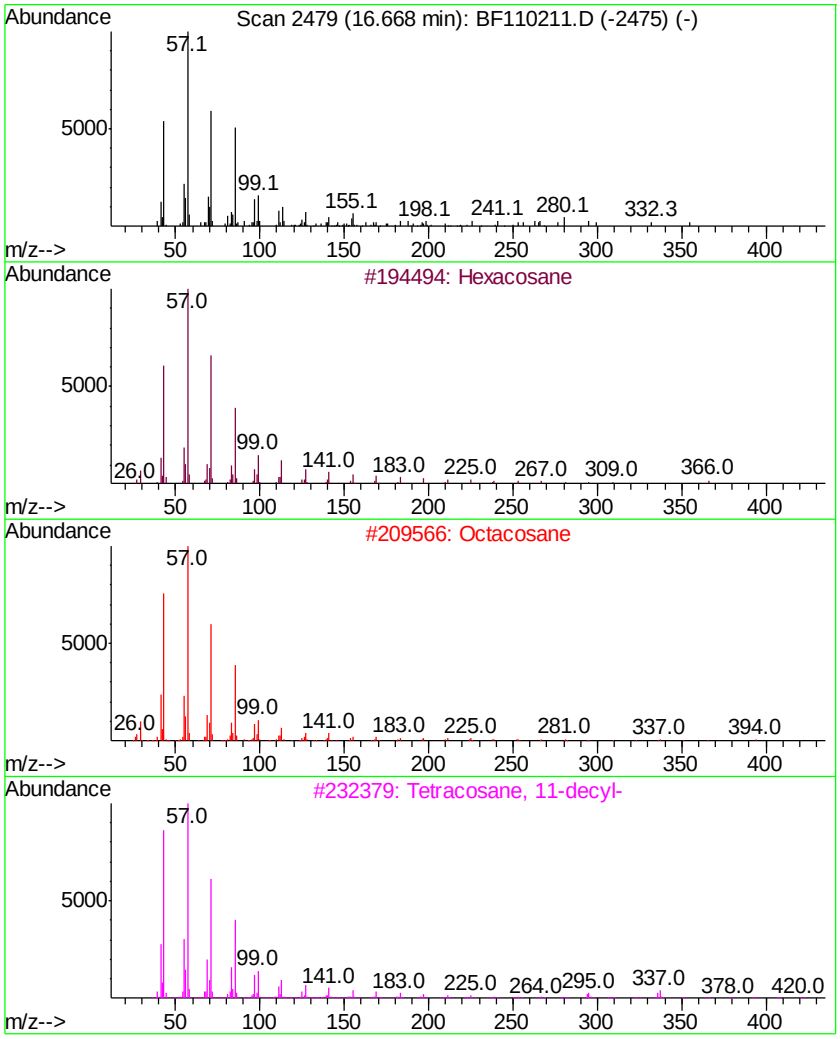
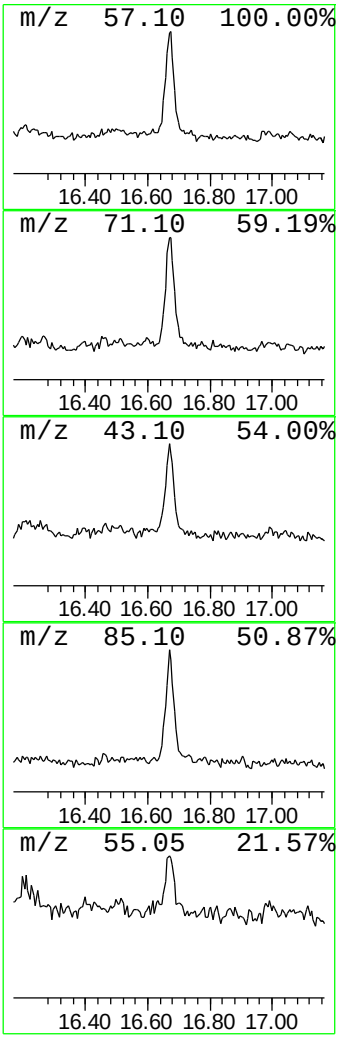
Peak Number 16 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	4.51 ng	178735	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Octacosane	394	C28H58	000630-02-4	86
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86
4	Nonadecane	268	C19H40	000629-92-5	80
5	Tetracosane	338	C24H50	000646-31-1	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102618\
Data File : BF110211.D
Acq On : 26 Oct 2018 15:56
Operator : JU/SJ
Sample : J5621-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-SB-01A

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...	2.32	11.5	ng	426513	1	6.97	743927	20.0
Acetic acid, 1,1-...	5.21	7.3	ng	270075	1	6.97	743927	20.0
unknown6.74	6.74	74.1	ng	2756570	1	6.97	743927	20.0
Decane	6.79	2.1	ng	78750	1	6.97	743927	20.0
Pentadecane, 2,6,...	10.91	2.1	ng	80781	4	11.50	772604	20.0
n-Hexadecanoic acid	12.01	3.1	ng	120731	4	11.50	772604	20.0
Octacosyl heptafl...	13.97	8.5	ng	323845	5	14.15	760310	20.0
Hexacosane	14.29	2.8	ng	107849	5	14.15	760310	20.0
Nonadecane	14.59	6.2	ng	235590	5	14.15	760310	20.0
Heneicosane	14.92	5.2	ng	205765	6	15.68	791831	20.0
Eicosane	16.13	6.9	ng	271512	6	15.68	791831	20.0
Octacosane	16.67	4.5	ng	178735	6	15.68	791831	20.0