LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109930.D
Acq On : 17 Oct 2018 19:54
Operator : JU/SJ
Sample : J5200-11 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

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-BF101518.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	2.293	31	35	44	rVB	319054	421301	15.26%	1.241%
2	5.198	525	529	534	rBV	92469	93386	3.38%	0.275%
3	5.587	591	595	598	rBV	2574092	2185473	79.18%	6.440%
4	6.587	760	765	770	rBV	2561273	2324735	84.22%	6.850%
5	6.739	787	791	794	rBV	2818946	2297114	83.22%	6.769%
6	6.975	827	831	834	rBV	2087708	1634224	59.21%	4.816%
7	7.128	854	857	861	rBV	1888782	1623472	58.82%	4.784%
8	7.534	922	926	929	rBV	1681753	1337325	48.45%	3.941%
9	8.257	1045	1049	1052	rBV	2621937	2147934	77.82%	6.329%
10	9.333	1228	1232	1235	rVB	2291975	2050623	74.29%	6.043%
11	9.722	1295	1298	1301	rVB	269939	200747	7.27%	0.592%
12	10.016	1344	1348	1352	rBV	2450399	2171723	78.68%	6.400%
13	10.422	1412	1417	1422	rVB2	24152	36828	1.33%	0.109%
14	10.563	1438	1441	1447	rVB	53330	45941	1.66%	0.135%
15	10.804	1478	1482	1485	rBV	1355282	1118424	40.52%	3.296%
16	10.922	1497	1502	1506	rVB4	22339	33485	1.21%	0.099%
17	11.510	1598	1602	1604	rBV	2121982	1904214	68.99%	5.611%
18	11.527	1604	1605	1609	rVV	328213	236722	8.58%	0.698%
19	11.580	1609	1614	1617	rVB	71371	61509	2.23%	0.181%
20	12.010	1684	1687	1690	rBV2	155734	188491	6.83%	0.555%
21	12.033	1690	1691	1695	rVB	85291	60507	2.19%	0.178%
22	12.121	1703	1706	1708	rBV2	66597	70571	2.56%	0.208%
23	12.139	1708	1709	1715	rVB	40208	35797	1.30%	0.105%
24	12.304	1733	1737	1739	rBV	35117	35699	1.29%	0.105%
25	12.327	1739	1741	1746	rVB5	28573	30309	1.10%	0.089%
26	12.557	1777	1780	1782	rBV	48532	46777	1.69%	0.138%
27	12.645	1792	1795	1799	rBV4	28628	34418	1.25%	0.101%
28	12.721	1805	1808	1811	rBV	395905	322941	11.70%	0.952%
29	12.804	1819	1822	1828	rBV4	75469	81539	2.95%	0.240%
30	12.951	1841	1847	1853	rBV	365406	391729	14.19%	1.154%
31	13.004	1853	1856	1860	rVB2	23405	28409	1.03%	0.084%
32	13.086	1867	1870	1874	rBV	1681761	1451092	52.57%	4.276%
33	13.163	1880	1883	1887	rBV4	31720	51586	1.87%	0.152%
34	13.274	1896	1902	1905	rVB	56540	73556	2.66%	0.217%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109930.D
Acq On : 17 Oct 2018 19:54
Operator : JU/SJ
Sample : J5200-11 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

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-BF101518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.345	1911	1914	1916	rVB	41425	33656	1.22%	0.099%
36	13.380	1917	1920	1923	rBV2	46038	46116	1.67%	0.136%
37	13.651	1963	1966	1968	rBV2	66902	50357	1.82%	0.148%
38	13.786	1986	1989	1993	rVB	37163	42361	1.53%	0.125%
39	13.974	2015	2021	2029	rBV5	186193	310324	11.24%	0.914%
40	14.151	2046	2051	2054	rBV	1994274	1900485	68.85%	5.600%
41	14.174	2054	2055	2060	rVB	180634	125899	4.56%	0.371%
42	14.298	2072	2076	2080	rBV	203997	219192	7.94%	0.646%
43	14.604	2124	2128	2131	rBV	357879	335170	12.14%	0.988%
44	14.921	2179	2182	2187	rBV	570890	561230	20.33%	1.654%
45	15.004	2193	2196	2199	rVB	90935	95464	3.46%	0.281%
46	15.215	2228	2232	2236	rBV	158833	262594	9.51%	0.774%
47	15.280	2239	2243	2249	rVB	701186	815708	29.55%	2.404%
48	15.539	2284	2287	2293	rVB	109780	166040	6.02%	0.489%
49	15.604	2295	2298	2304	rVB	129486	166354	6.03%	0.490%
50	15.680	2305	2311	2322	rBV2	1917908	2760168	100.00%	8.134%
51	16.151	2386	2391	2397	rBV	490624	731152	26.49%	2.155%
52	16.692	2477	2483	2490	rBV	237248	484649	17.56%	1.428%

Sum of corrected areas: 33935520

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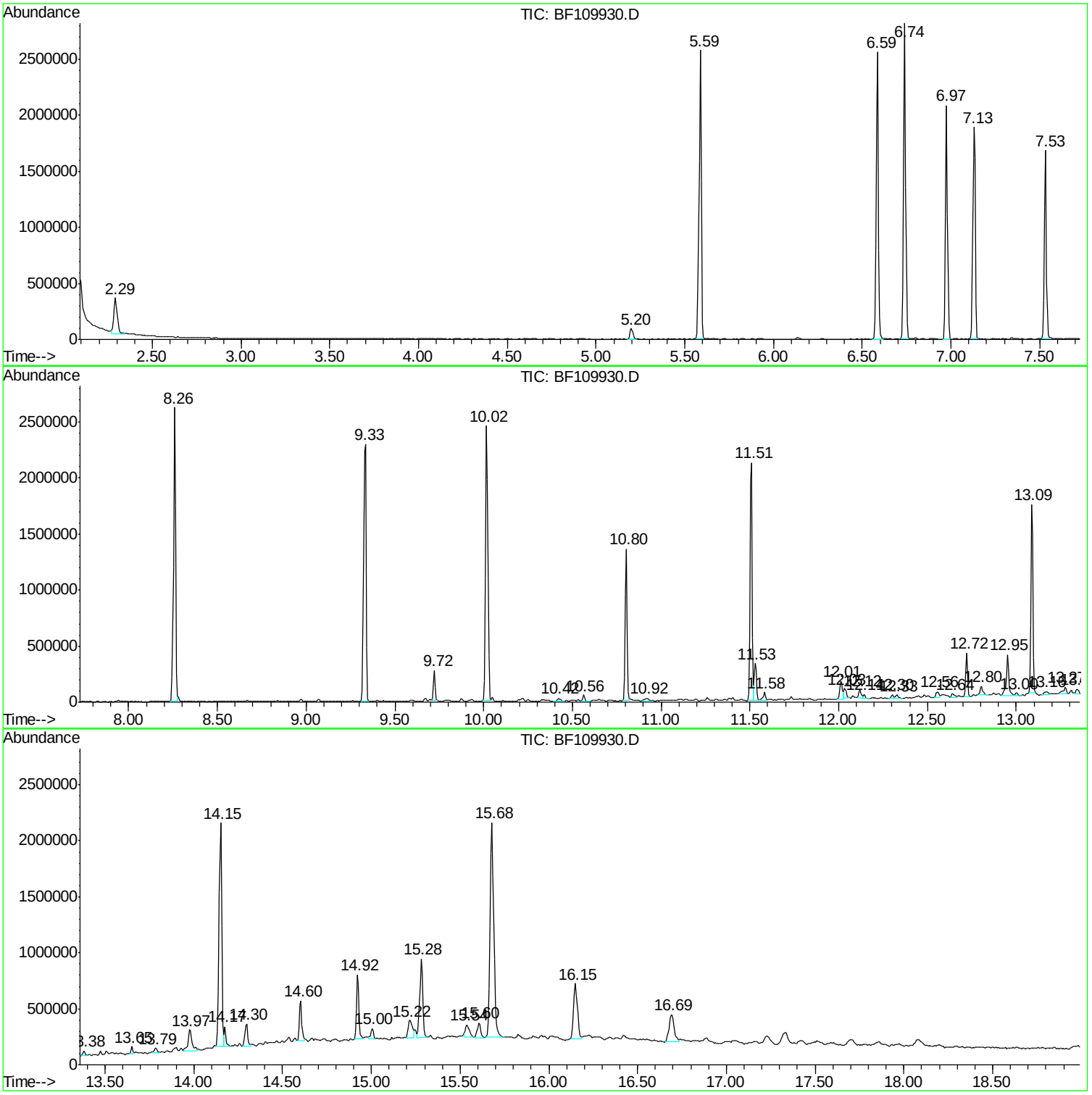
Sample : J5200-11 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109930.D
Acq On : 17 Oct 2018 19:54
Operator : JU/SJ
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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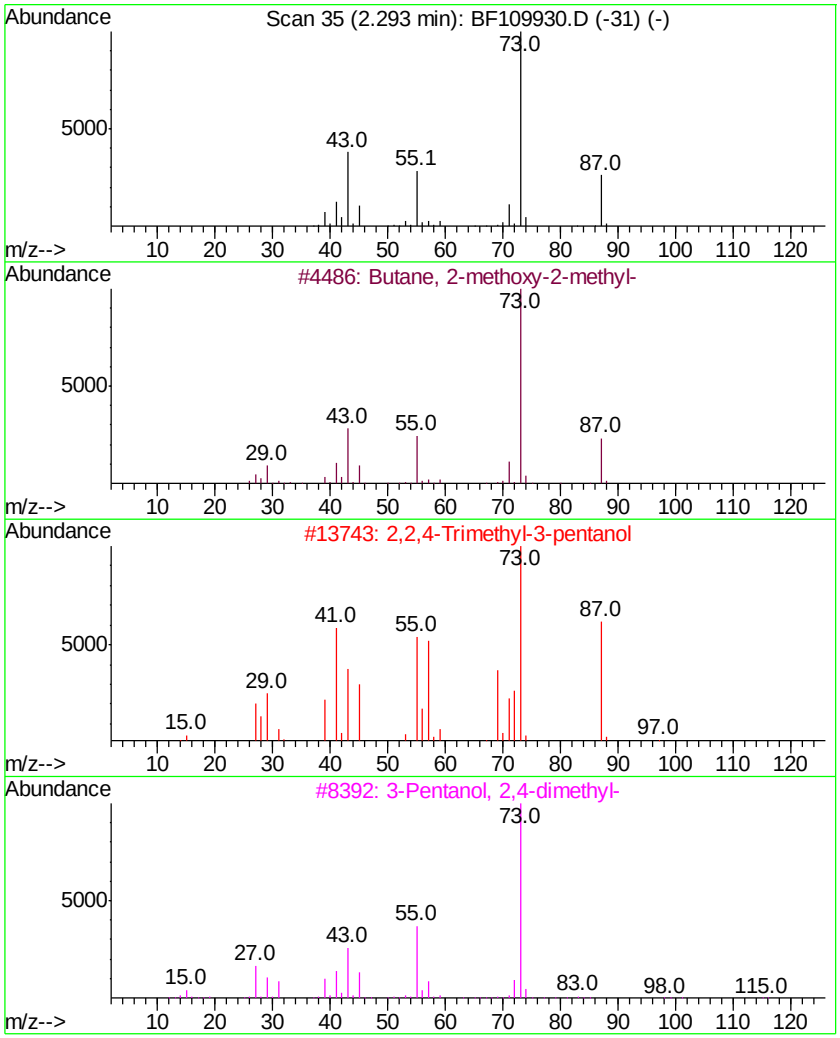
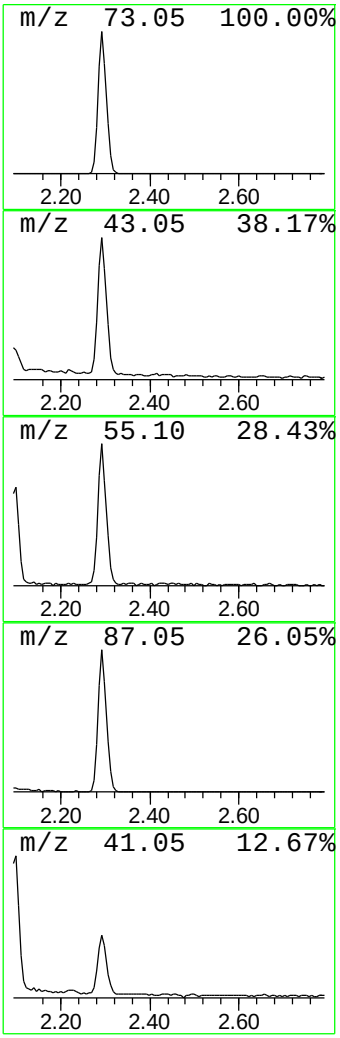
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	5.16 ng	421301	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	39
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109930.D
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Operator : JU/SJ
Sample : J5200-11 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

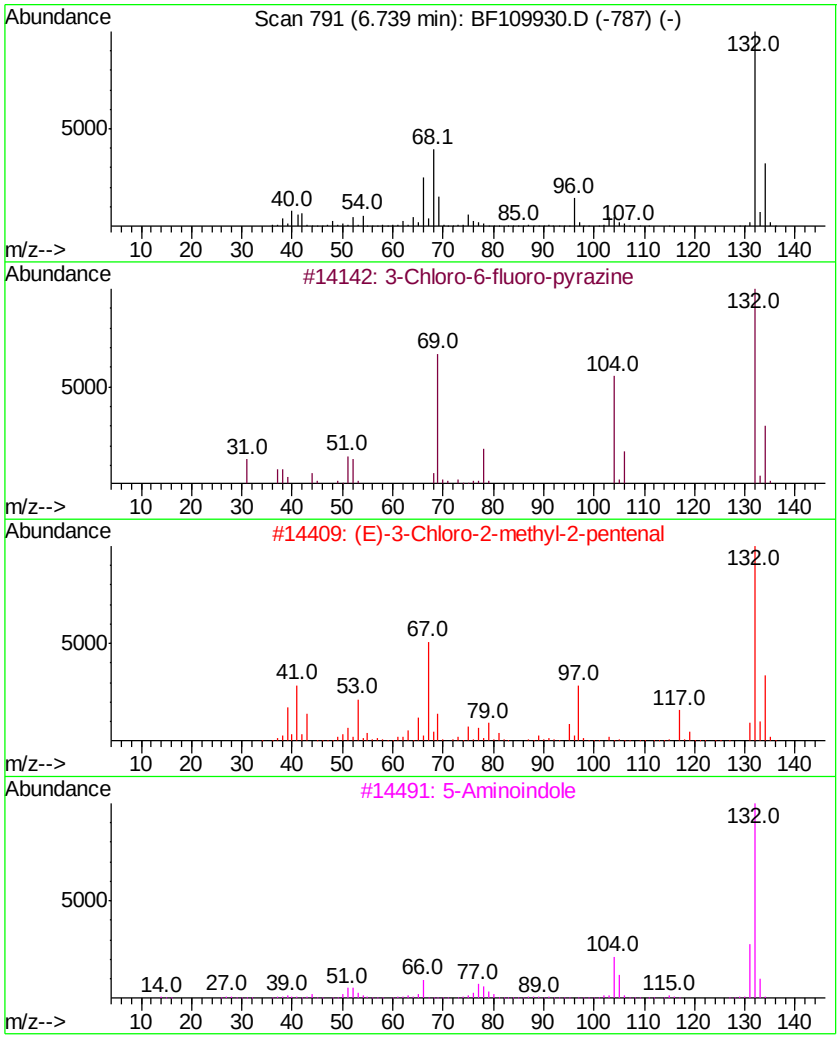
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

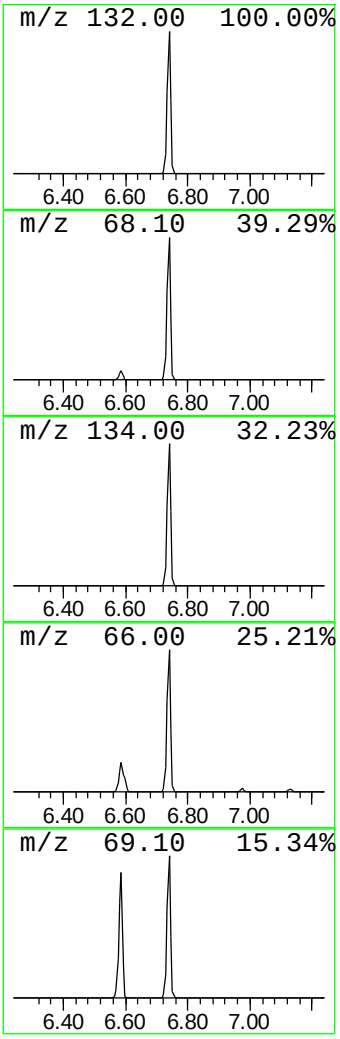
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	28.11 ng	2297110	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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
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





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
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Acq On : 17 Oct 2018 19:54
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Sample : J5200-11 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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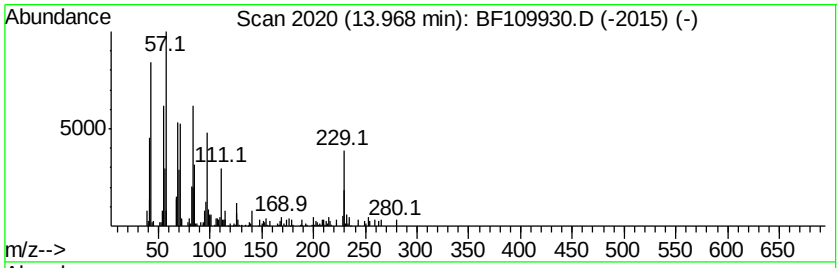
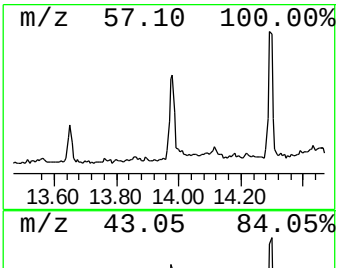
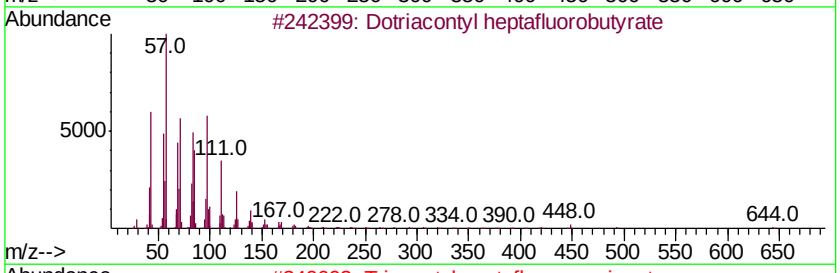
Peak Number 4 Dotriacontyl heptafluorobut... Concentration Rank 9

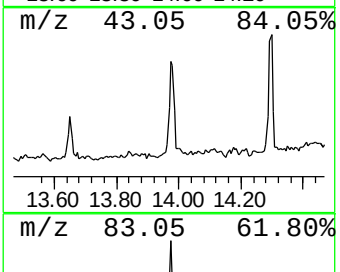
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.27 ng	310324	Chrysene-d12	14.15

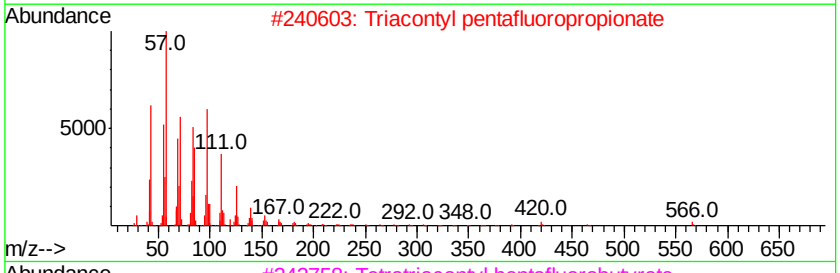
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	90
2	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	90
3	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	90
4	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	90
5	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	90

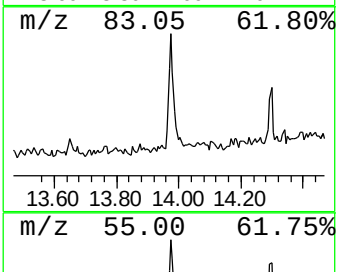


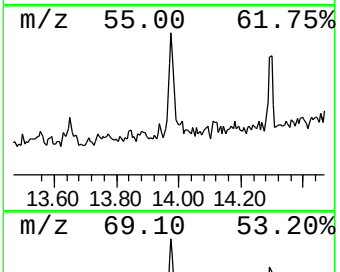


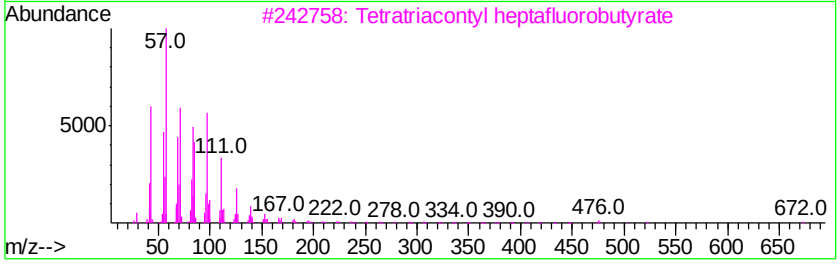


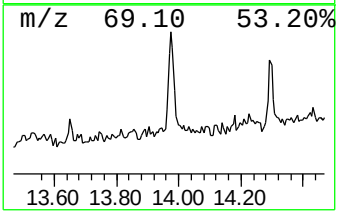












Library Search Compound Report

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

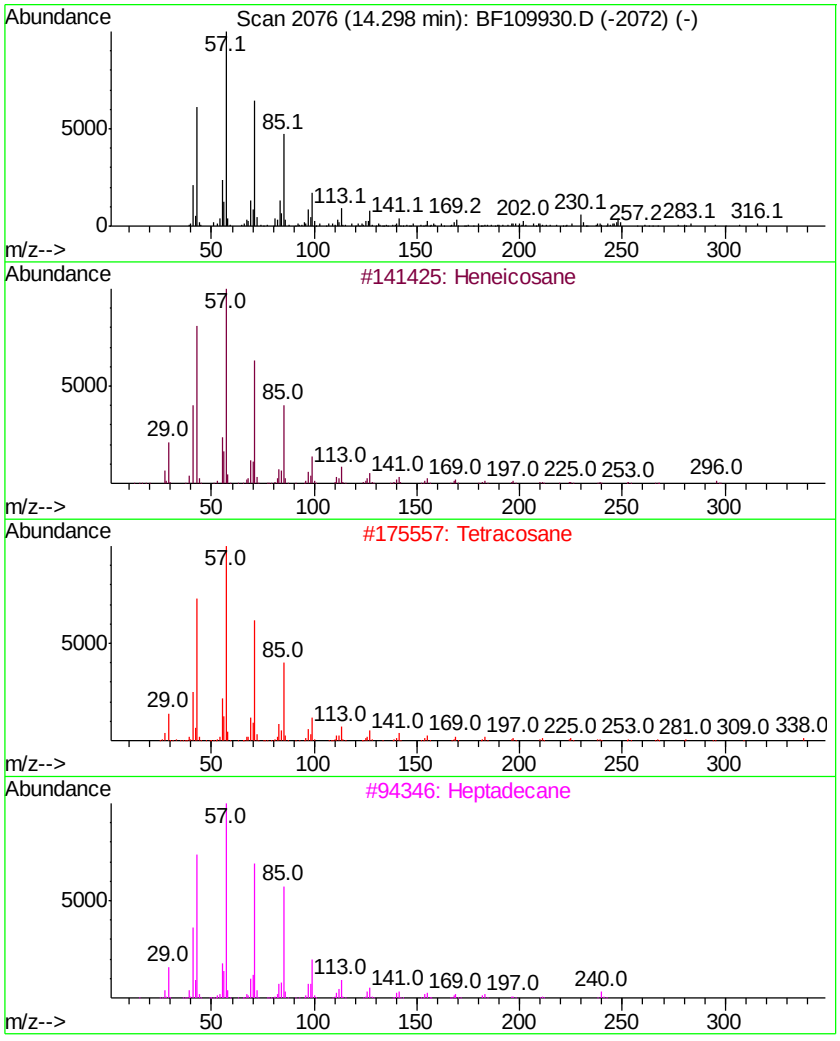
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

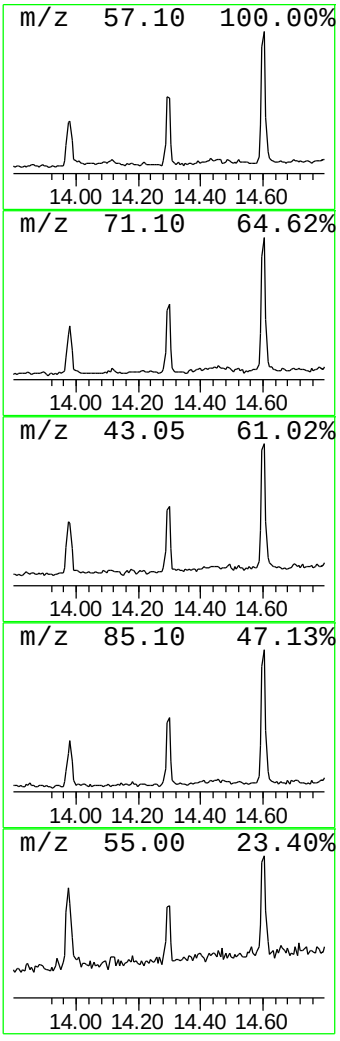
****

Peak Number 5 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	2.31 ng	219192	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	83
2	Tetracosane	338	C24H50	000646-31-1	83
3	Heptadecane	240	C17H36	000629-78-7	83
4	Eicosane	282	C20H42	000112-95-8	80
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	80





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Misc :
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Instrument : BNA_F
ClientSampleId : OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

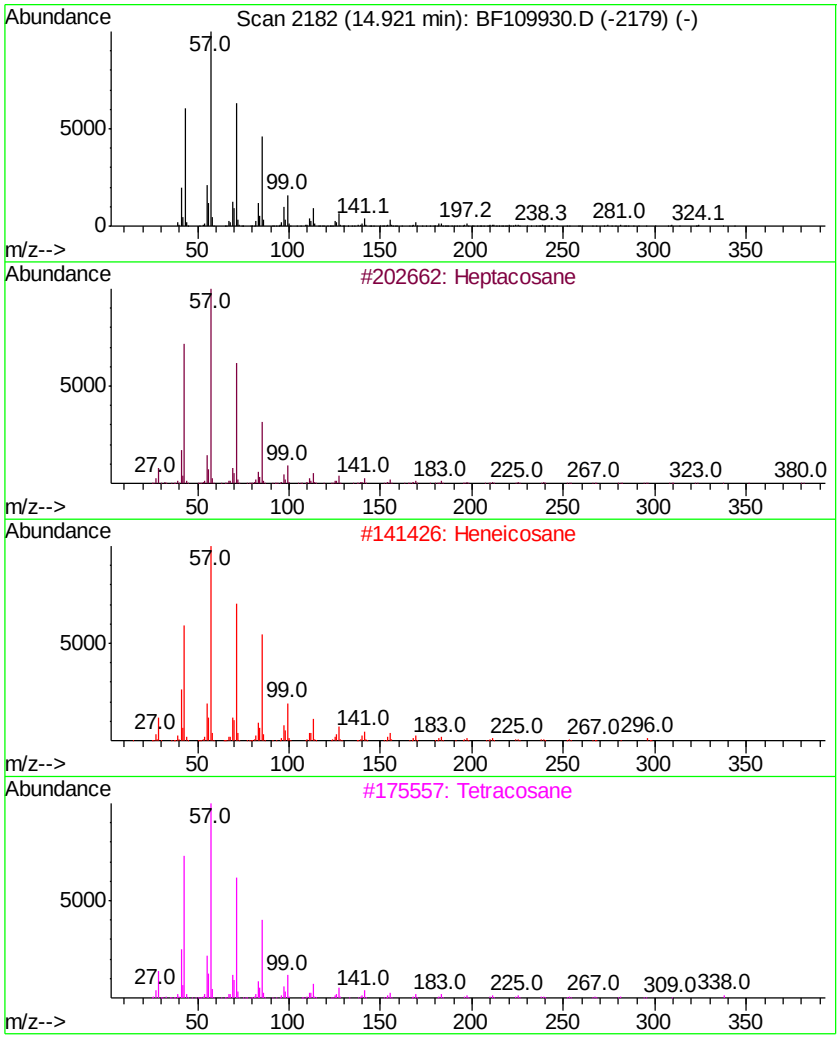
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

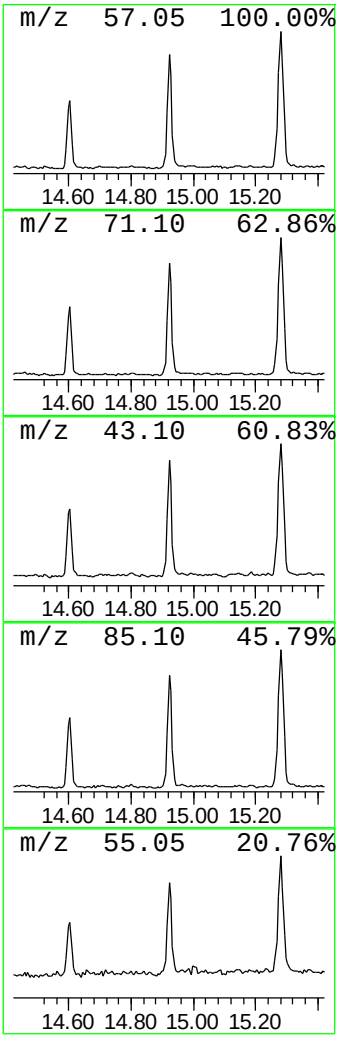
****

Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.07 ng	561230	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptadecane	240	C17H36	000629-78-7	87
5	Nonadecane	268	C19H40	000629-92-5	87





Library Search Compound Report

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Data File : BF109930.D
Acq On : 17 Oct 2018 19:54
Operator : JU/SJ
Sample : J5200-11 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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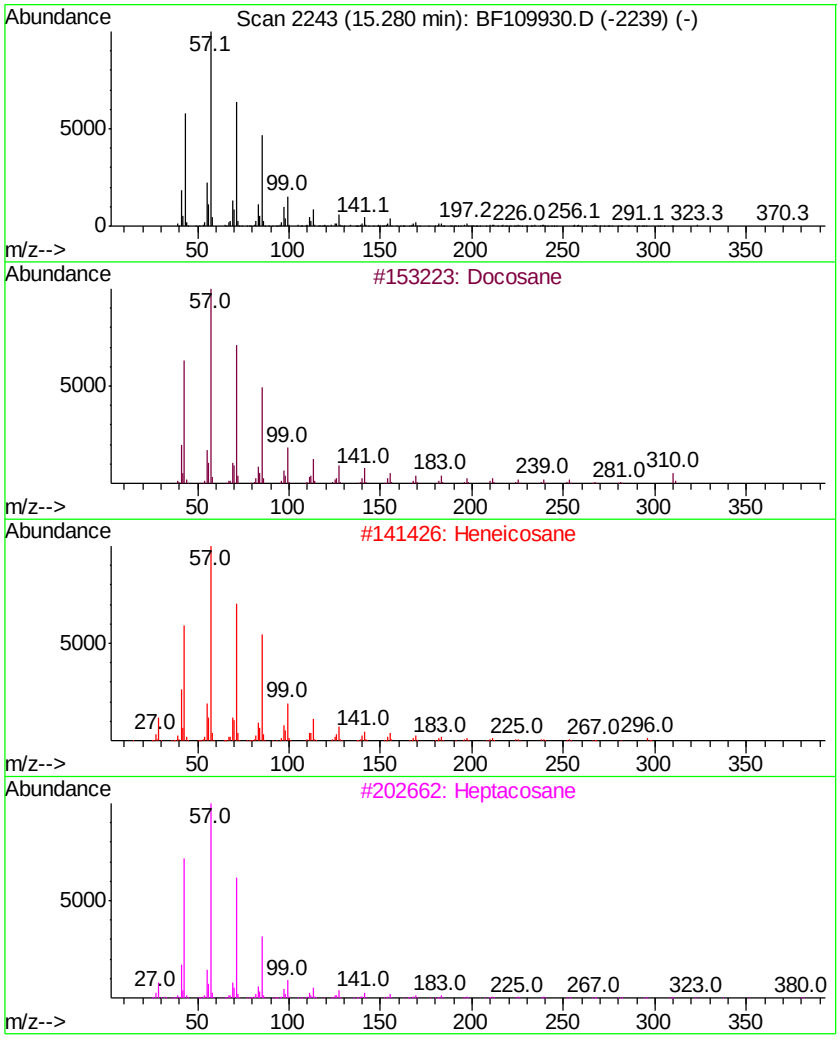
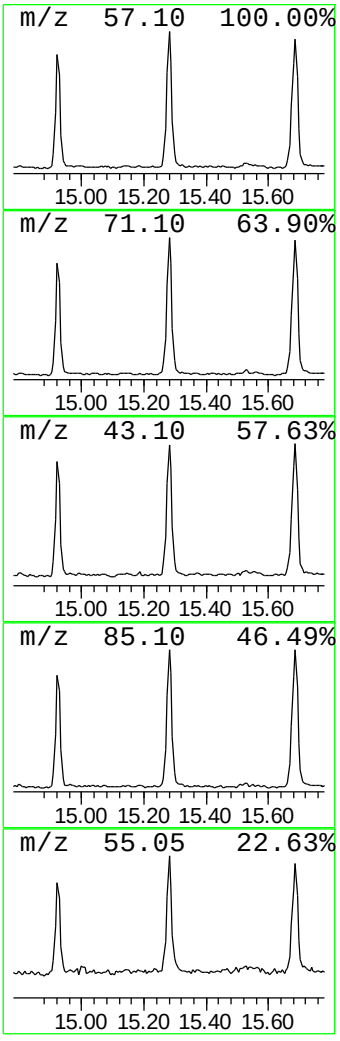
Peak Number 8 Docosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	5.91 ng	815708	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	96
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane	394	C28H58	000630-02-4	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109930.D
Acq On : 17 Oct 2018 19:54
Operator : JU/SJ
Sample : J5200-11 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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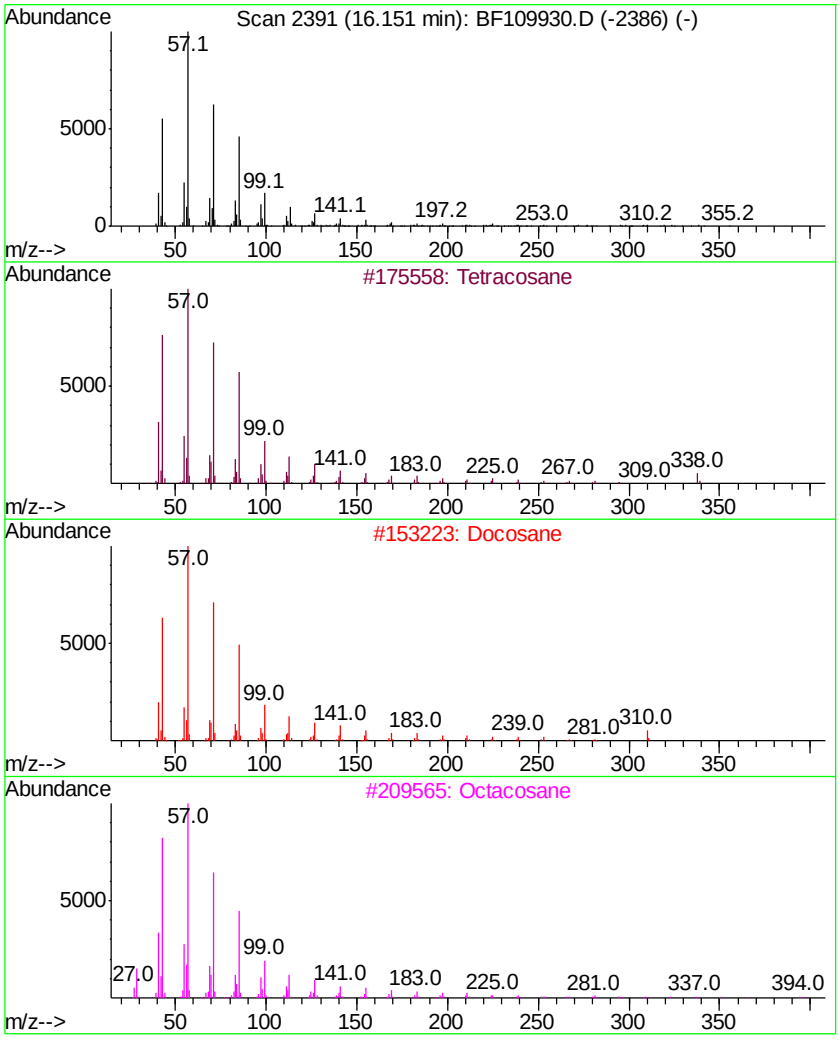
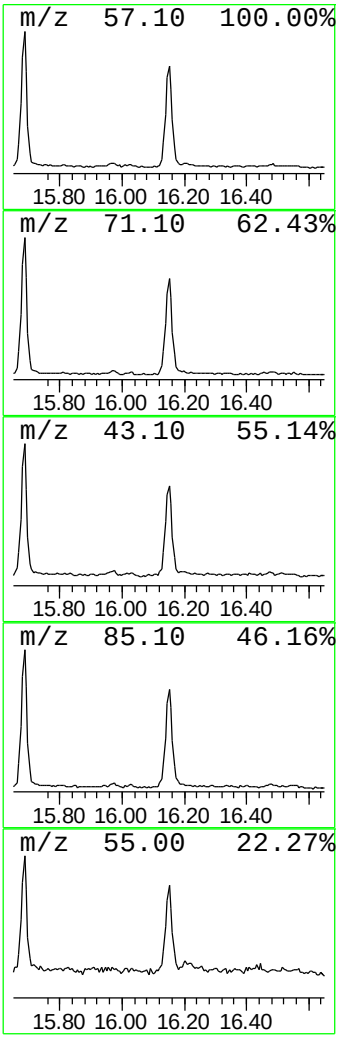
Peak Number 9 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	5.30 ng	731152	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Docosane	310	C22H46	000629-97-0	92
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109930.D
Acq On : 17 Oct 2018 19:54
Operator : JU/SJ
Sample : J5200-11 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

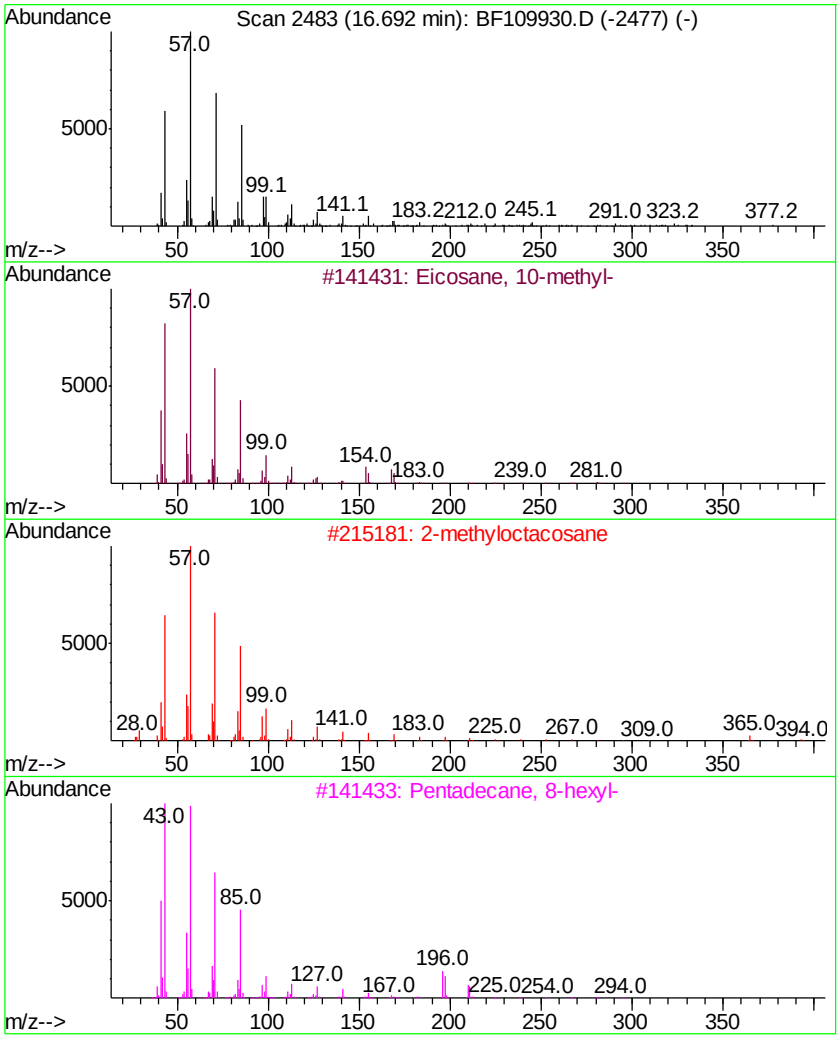
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

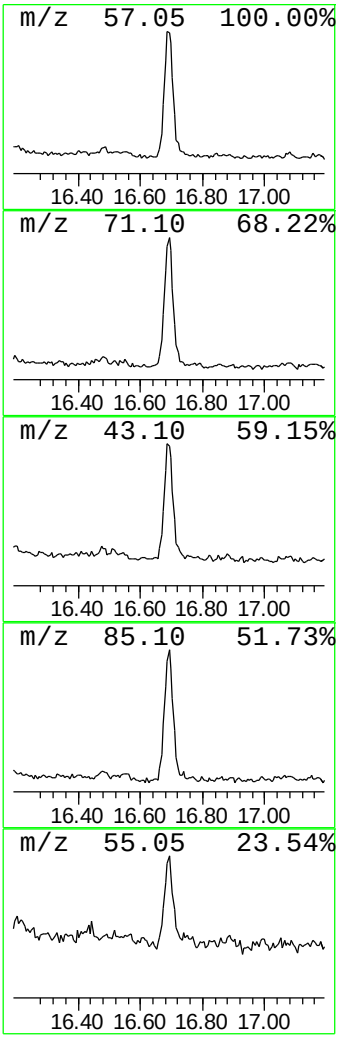
****

Peak Number 10 Eicosane, 10-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	3.51 ng	484649	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	87
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
5	Tetracosane	338	C24H50	000646-31-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101718\
Data File : BF109930.D
Acq On : 17 Oct 2018 19:54
Operator : JU/SJ
Sample : J5200-11 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-101618-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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...	2.29	5.2	ng	421301	1	6.97	1634220	20.0
unknown6.74	6.74	28.1	ng	2297110	1	6.97	1634220	20.0
Dotriacontyl hept...	13.97	3.3	ng	310324	5	14.15	1900490	20.0
Heneicosane	14.30	2.3	ng	219192	5	14.15	1900490	20.0
Heptacosane	14.92	4.1	ng	561230	6	15.68	2760170	20.0
Docosane	15.28	5.9	ng	815708	6	15.68	2760170	20.0
Tetracosane	16.15	5.3	ng	731152	6	15.68	2760170	20.0
Eicosane, 10-methyl-	16.69	3.5	ng	484649	6	15.68	2760170	20.0