LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110561.D
Acq On : 7 Nov 2018 17:53
Operator : JU/SJ
Sample : J5762-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-110518

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	2.234	21	25	42	rVB	138768	237605	25.23%	2.203%
2	5.175	522	525	535	rBV	23654	31186	3.31%	0.289%
3	5.569	588	592	603	rBV	816302	838404	89.04%	7.772%
4	6.569	759	762	781	rBV	888236	940301	99.86%	8.717%
5	6.716	784	787	795	rBV	1075872	924401	98.17%	8.569%
6	6.951	823	827	833	rBV	516847	454547	48.27%	4.214%
7	7.104	849	853	863	rBV	788333	696052	73.92%	6.452%
8	7.510	919	922	933	rBV	494608	545375	57.92%	5.056%
9	8.233	1041	1045	1051	rBV	535404	529657	56.25%	4.910%
10	8.504	1086	1091	1093	rBV4	7463	11254	1.20%	0.104%
11	8.557	1097	1100	1105	rBV4	6206	11836	1.26%	0.110%
12	8.763	1131	1135	1137	rBV2	11795	10891	1.16%	0.101%
13	8.969	1165	1170	1173	rBV5	11115	13632	1.45%	0.126%
14	9.304	1223	1227	1236	rBV	1063794	941642	100.00%	8.729%
15	9.380	1236	1240	1243	rVB3	24612	29034	3.08%	0.269%
16	9.698	1289	1294	1300	rBV	105849	124477	13.22%	1.154%
17	9.845	1316	1319	1322	rBV2	17736	17318	1.84%	0.161%
18	9.892	1324	1327	1330	rVB2	26256	23541	2.50%	0.218%
19	9.992	1341	1344	1353	rVB	570176	514286	54.62%	4.767%
20	10.298	1394	1396	1401	rBV6	6640	11290	1.20%	0.105%
21	10.392	1407	1412	1415	rVB4	11083	13467	1.43%	0.125%
22	10.622	1447	1451	1454	rBV3	10275	12757	1.35%	0.118%
23	10.786	1475	1479	1491	rBV	371730	402802	42.78%	3.734%
24	10.886	1491	1496	1503	rVB	13024	20313	2.16%	0.188%
25	11.486	1594	1598	1610	rBV	437783	423243	44.95%	3.924%
26	11.851	1658	1660	1664	rVB	38143	34191	3.63%	0.317%
27	11.986	1681	1683	1688	rBV2	25044	31861	3.38%	0.295%
28	12.539	1774	1777	1778	rBV	80639	60572	6.43%	0.562%
29	12.557	1778	1780	1783	rVB	133265	114920	12.20%	1.065%
30	12.645	1792	1795	1798	rVB	32284	25869	2.75%	0.240%
31	12.704	1802	1805	1808	rBV	13365	13711	1.46%	0.127%
32	12.939	1843	1845	1850	rVB3	15400	15992	1.70%	0.148%
33	13.063	1863	1866	1870	rBV	778681	692726	73.57%	6.422%
34	13.368	1915	1918	1923	rBV5	8795	17643	1.87%	0.164%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J5762-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-110518

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	13.568	1948	1952	1954	rBV5	9994	16959	1.80%	0.157%
36	13.615	1958	1960	1963	rVB4	14331	12559	1.33%	0.116%
37	13.945	2012	2016	2020	rBV2	67040	90593	9.62%	0.840%
38	14.133	2044	2048	2055	rBV	533212	549371	58.34%	5.093%
39	14.262	2067	2070	2074	rBV	34712	36007	3.82%	0.334%
40	14.562	2118	2121	2125	rBV	74478	86946	9.23%	0.806%
41	14.880	2171	2175	2180	rBV2	143390	188006	19.97%	1.743%
42	15.233	2232	2235	2239	rVB	144786	165040	17.53%	1.530%
43	15.633	2299	2303	2305	rBV	121802	181390	19.26%	1.682%
44	15.662	2305	2308	2314	rVB	327021	408499	43.38%	3.787%
45	16.086	2376	2380	2387	rVB2	111106	172439	18.31%	1.599%
46	16.615	2467	2470	2477	rVB2	56830	92763	9.85%	0.860%

Sum of corrected areas: 10787368

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Misc :
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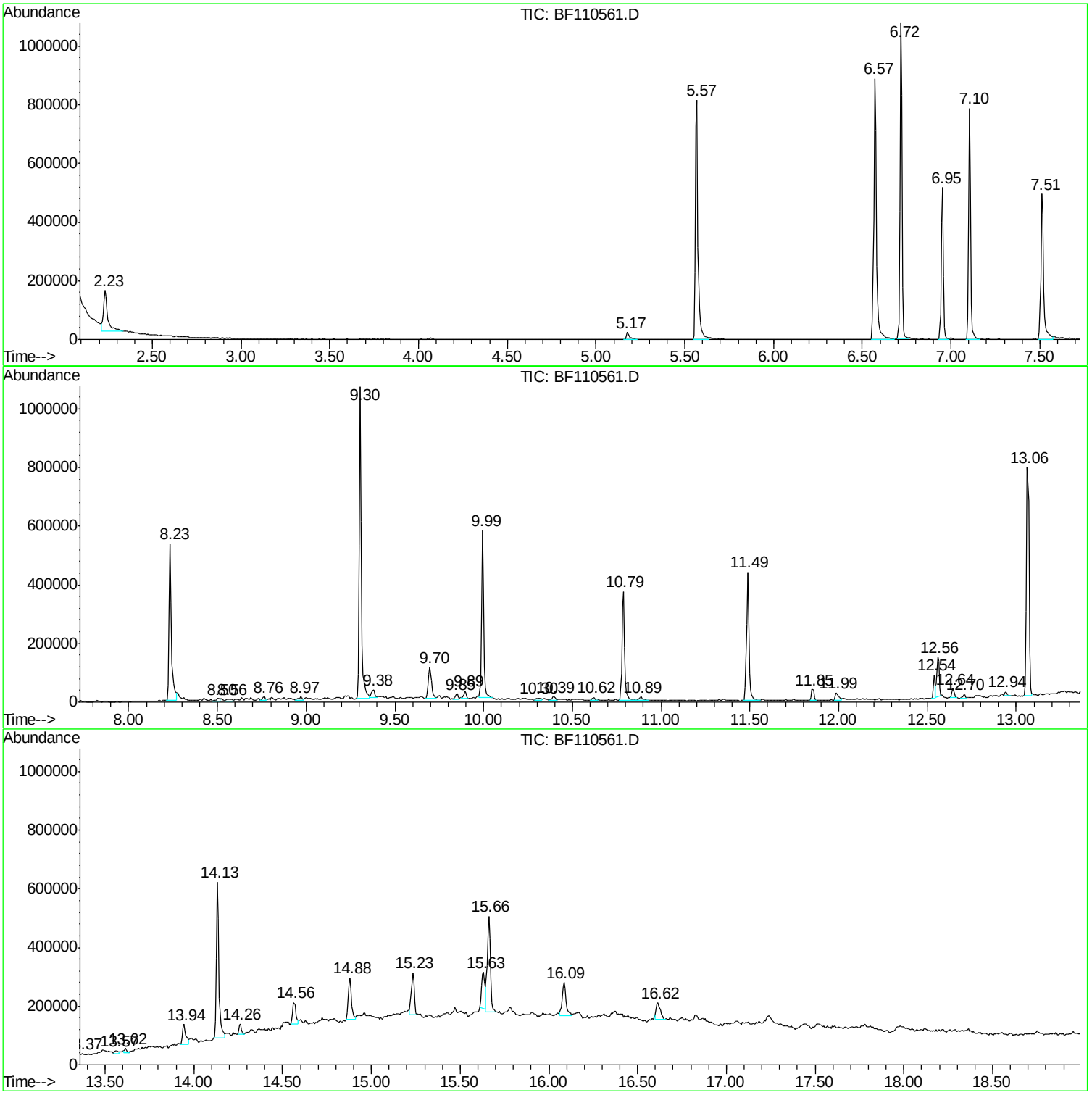
Instrument :
BNA_F
ClientSampleId :
BU-02-110518

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110561.D
Acq On : 7 Nov 2018 17:53
Operator : JU/SJ
Sample : J5762-03 2X
Misc :
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Instrument : BNA_F
ClientSampleId : BU-02-110518

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

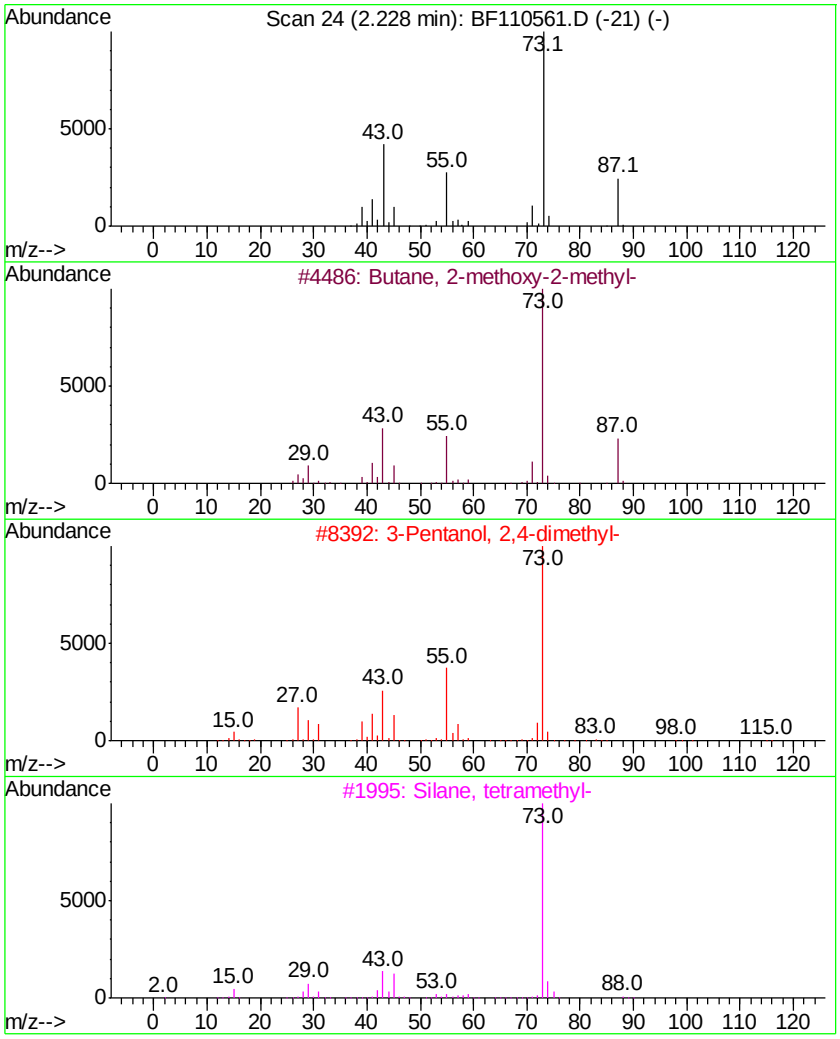
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

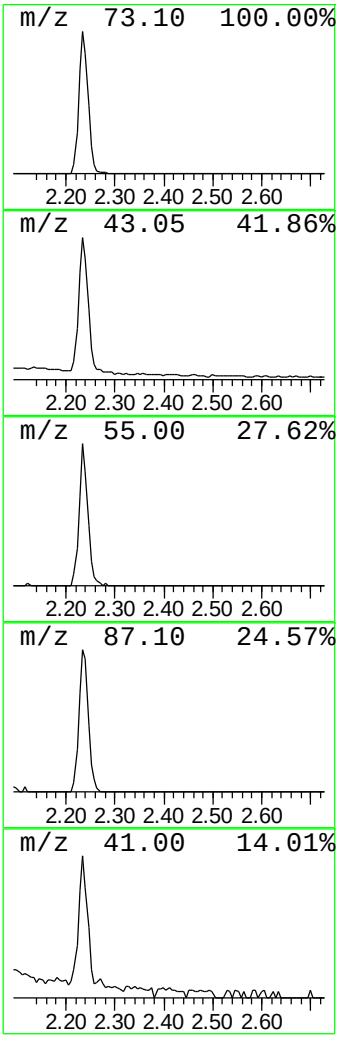
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	10.45 ng	237605	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	72
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110561.D
Acq On : 7 Nov 2018 17:53
Operator : JU/SJ
Sample : J5762-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-110518

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

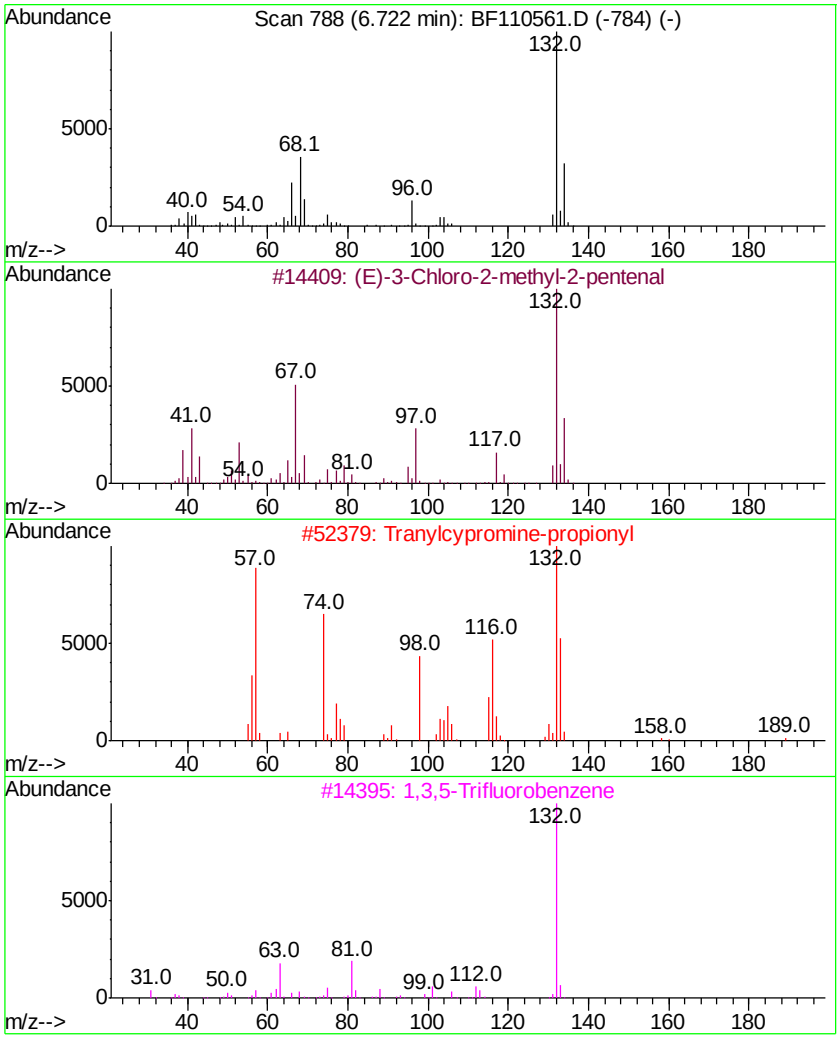
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

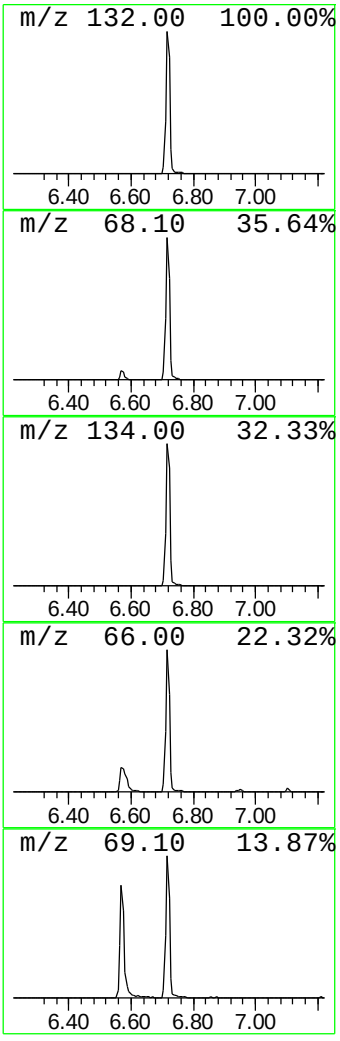
****

Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	40.67 ng	924401	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110561.D
Acq On : 7 Nov 2018 17:53
Operator : JU/SJ
Sample : J5762-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-110518

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

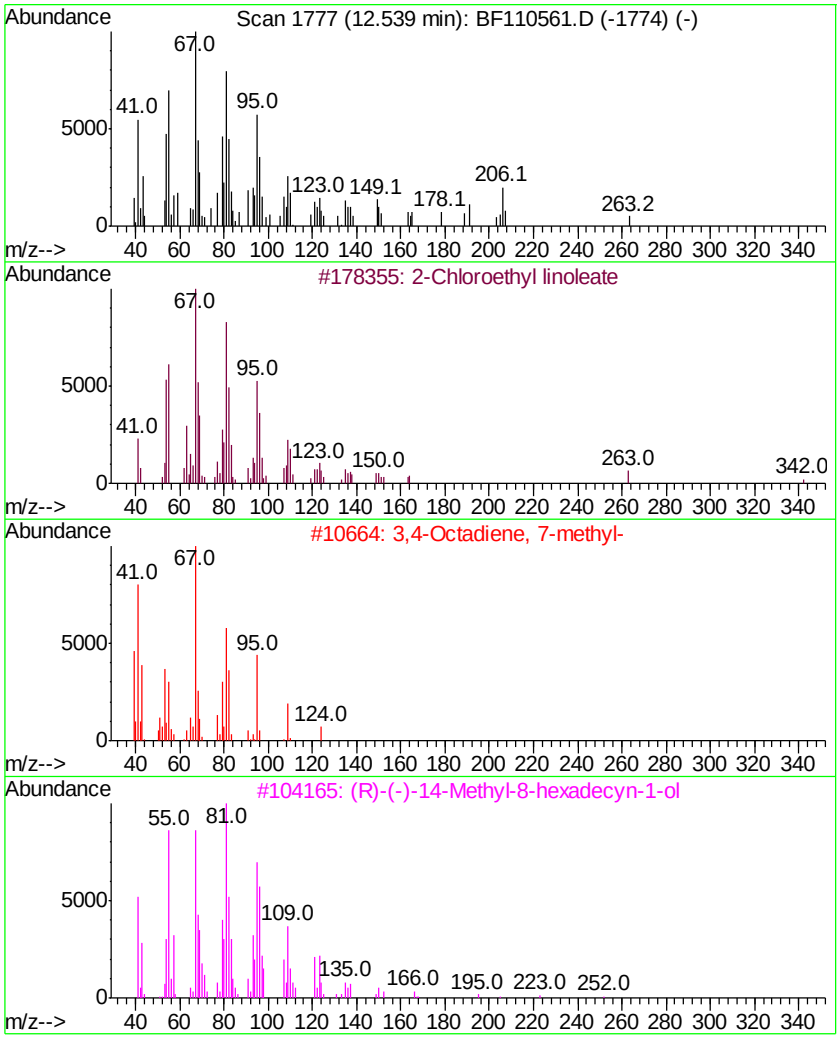
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

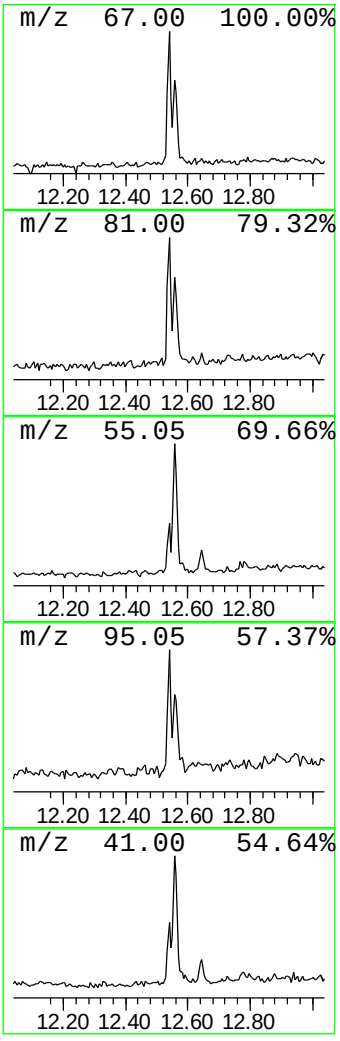
****

Peak Number 4 2-Chloroethyl linoleate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	2.86 ng	60572	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	90
2	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	81
3	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	064566-18-3	76
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	76
5	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	70





Library Search Compound Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-110518

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

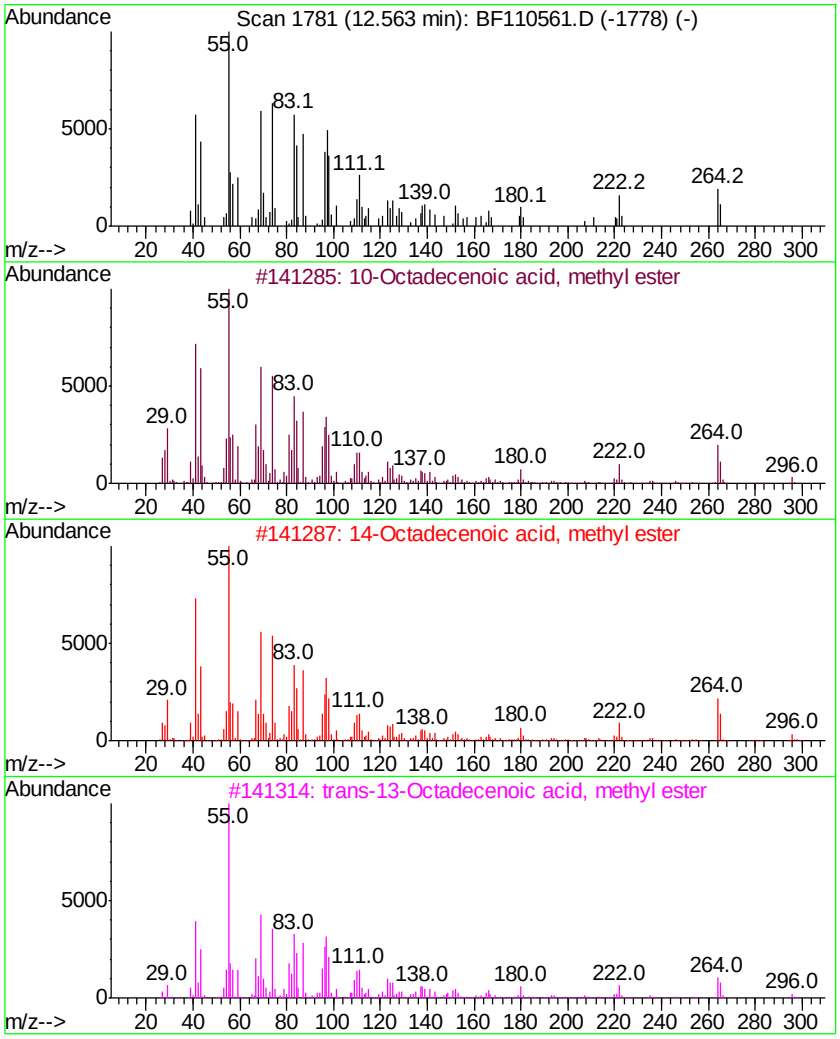
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

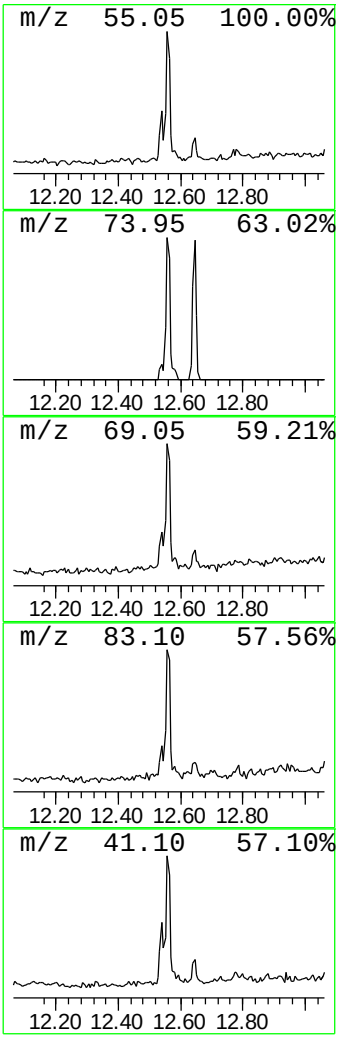
****

Peak Number 5 10-Octadecenoic acid, methy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	5.43 ng	114920	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	87
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	83
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	83





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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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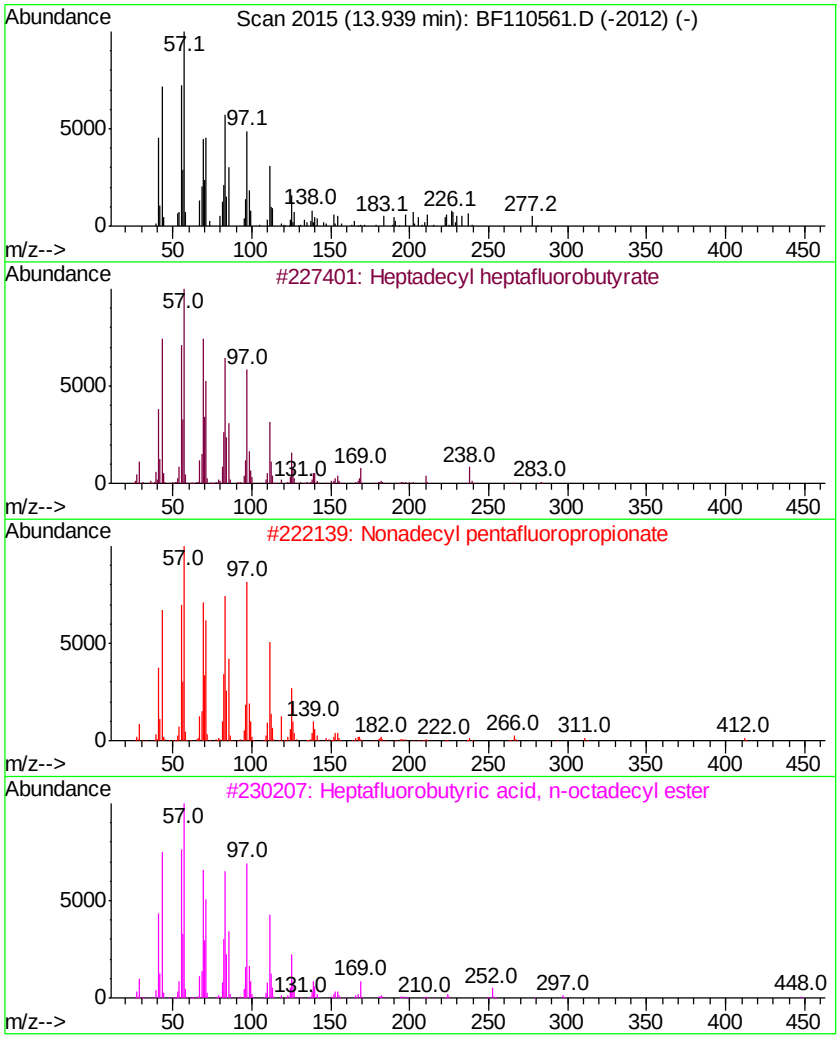
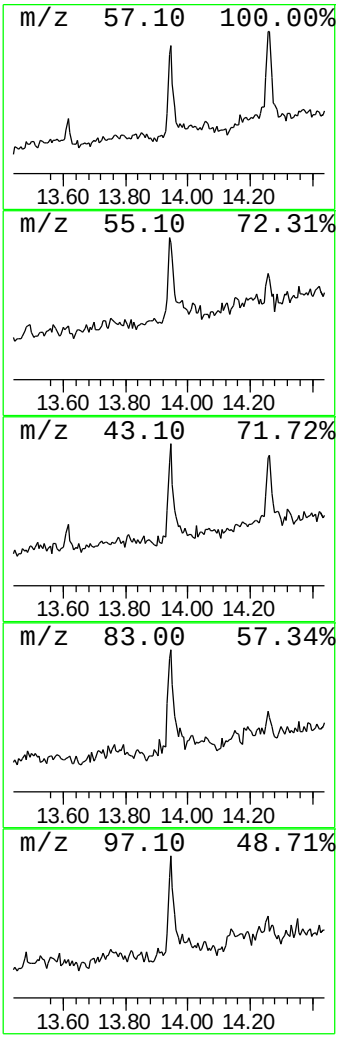
****

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	3.30 ng	90593	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	83
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76
5	17-Pentatriacontene	491	C35H70	006971-40-0	74





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Misc :
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Instrument : BNA_F
ClientSampleId : BU-02-110518

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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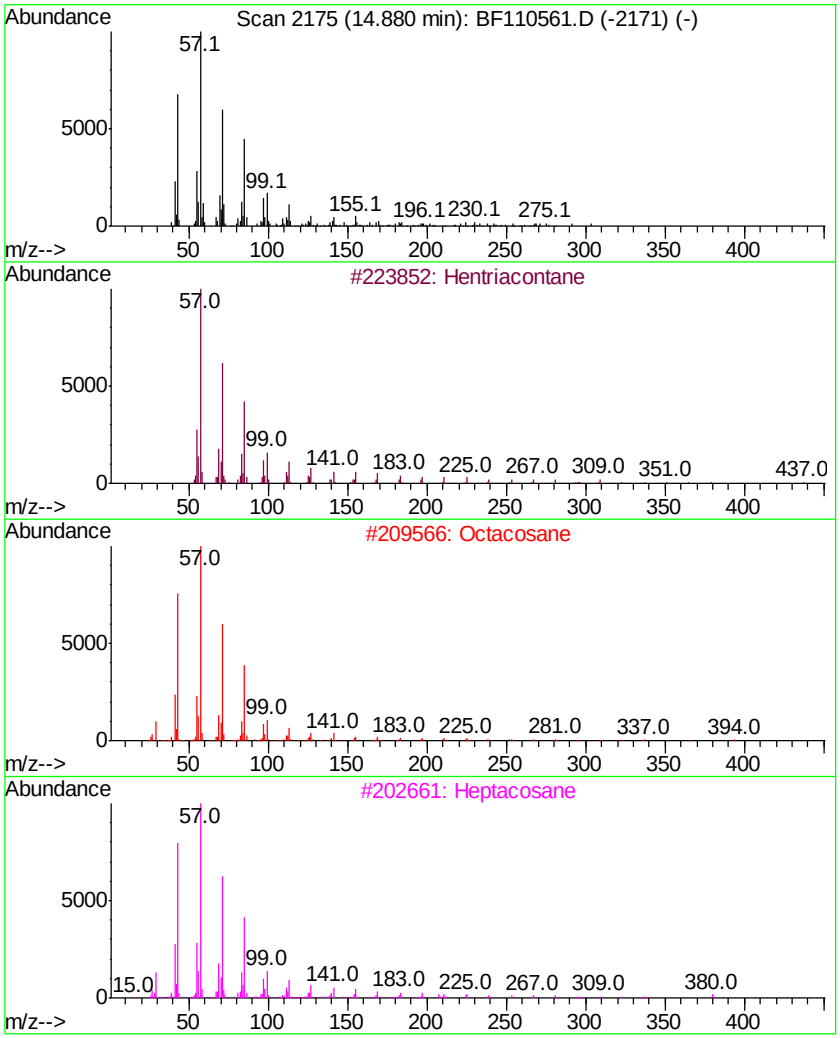
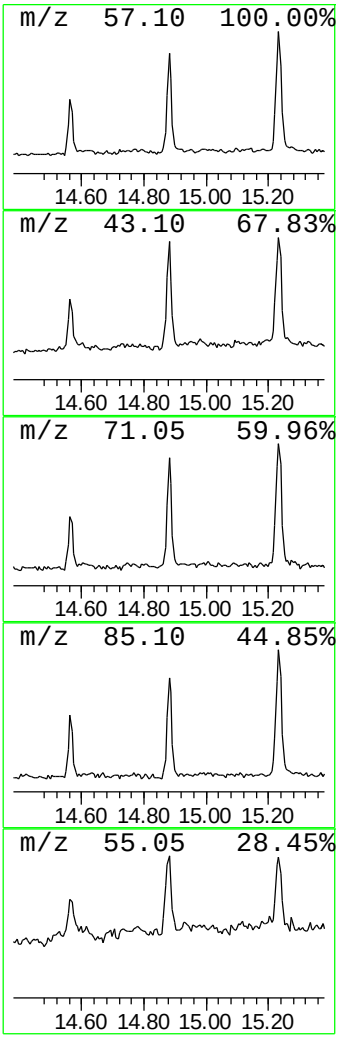
Peak Number 8 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	6.84 ng	188006	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Heptacosane	380	C27H56	000593-49-7	87
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	81
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80





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Misc :
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Instrument : BNA_F
ClientSampleId : BU-02-110518

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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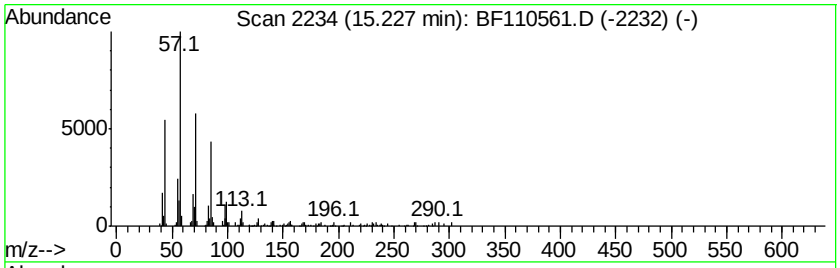
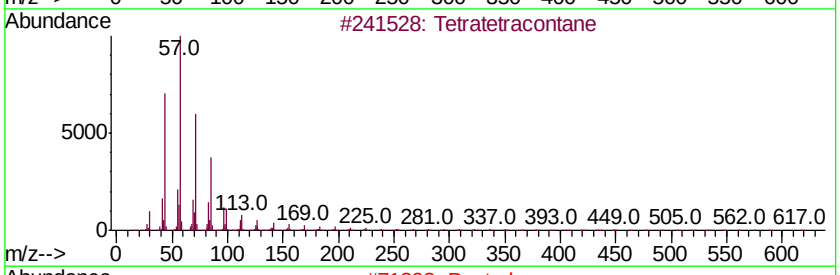
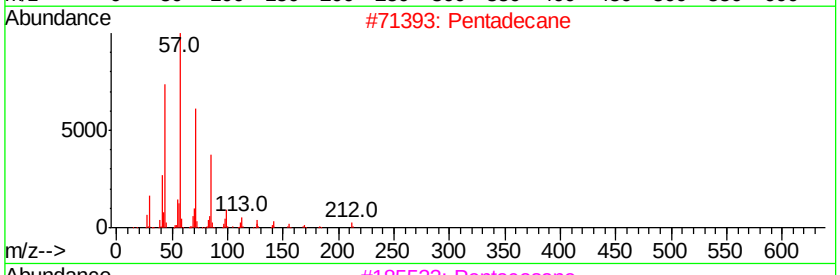
Peak Number 9 Tetratetracontane Concentration Rank 5

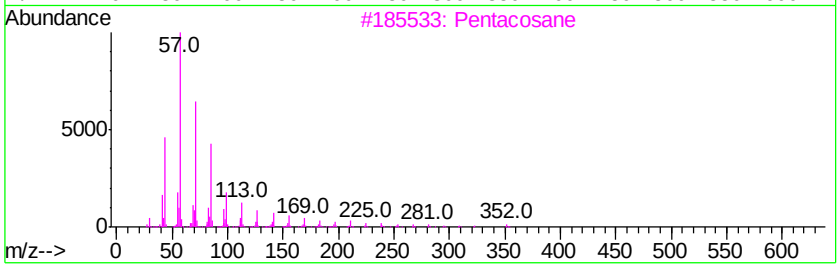
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	8.08 ng	165040	Perylene-d12	15.66

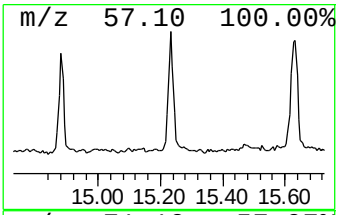
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Pentacosane	352	C25H52	000629-99-2	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	83

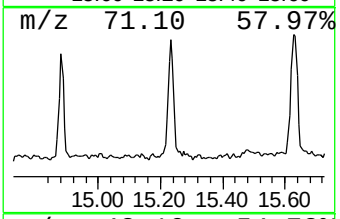


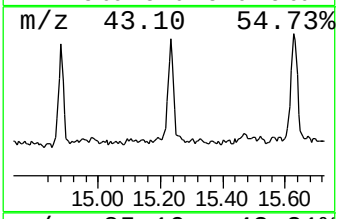


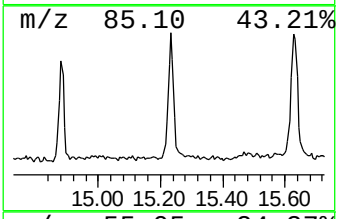


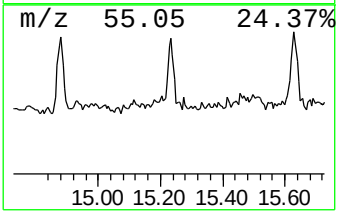












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110561.D
Acq On : 7 Nov 2018 17:53
Operator : JU/SJ
Sample : J5762-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-110518

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

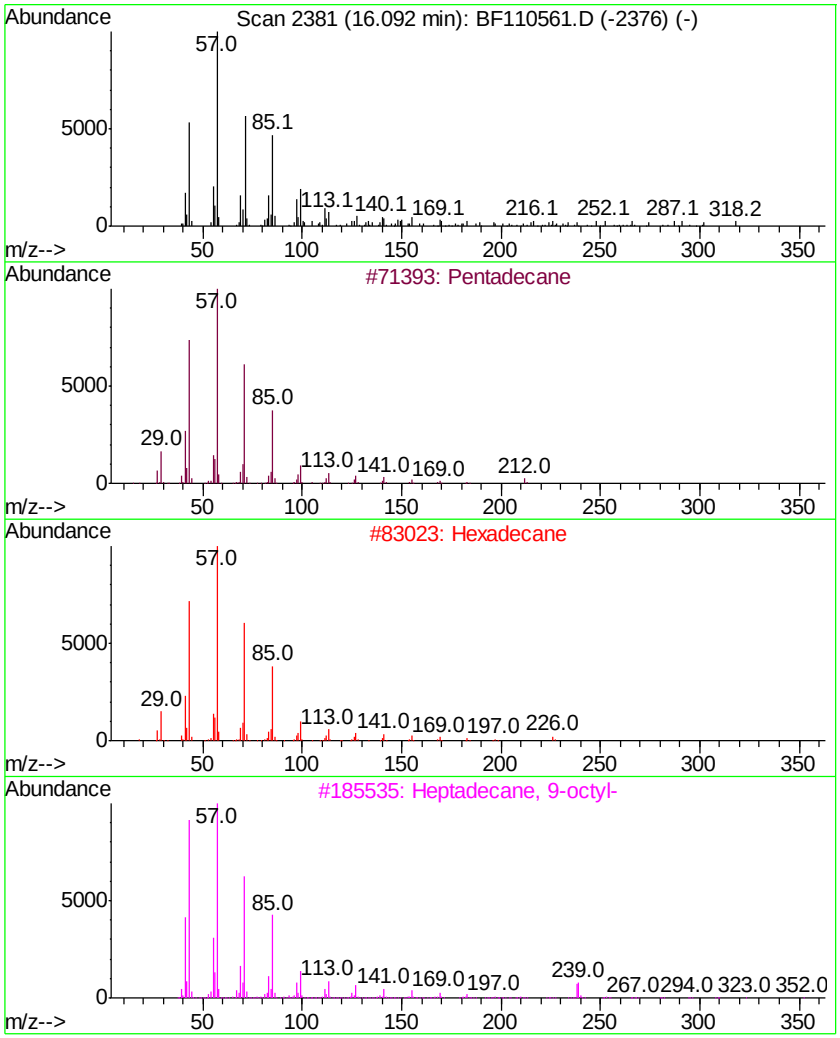
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

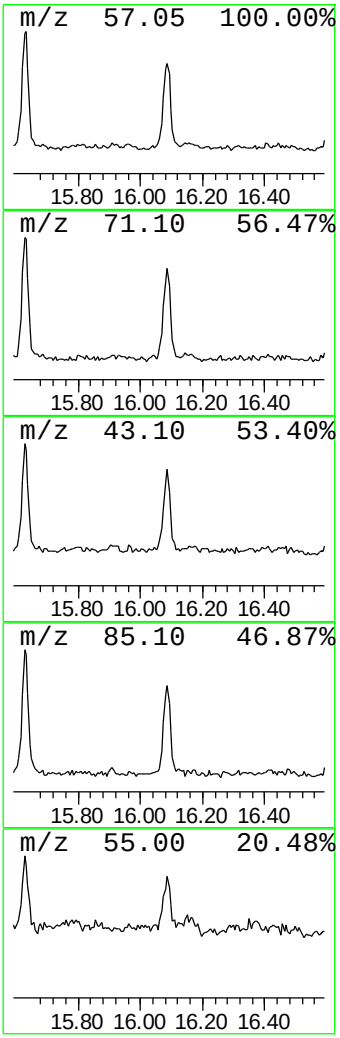
****

Peak Number 10 Pentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	8.44 ng	172439	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110561.D
Acq On : 7 Nov 2018 17:53
Operator : JU/SJ
Sample : J5762-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-110518

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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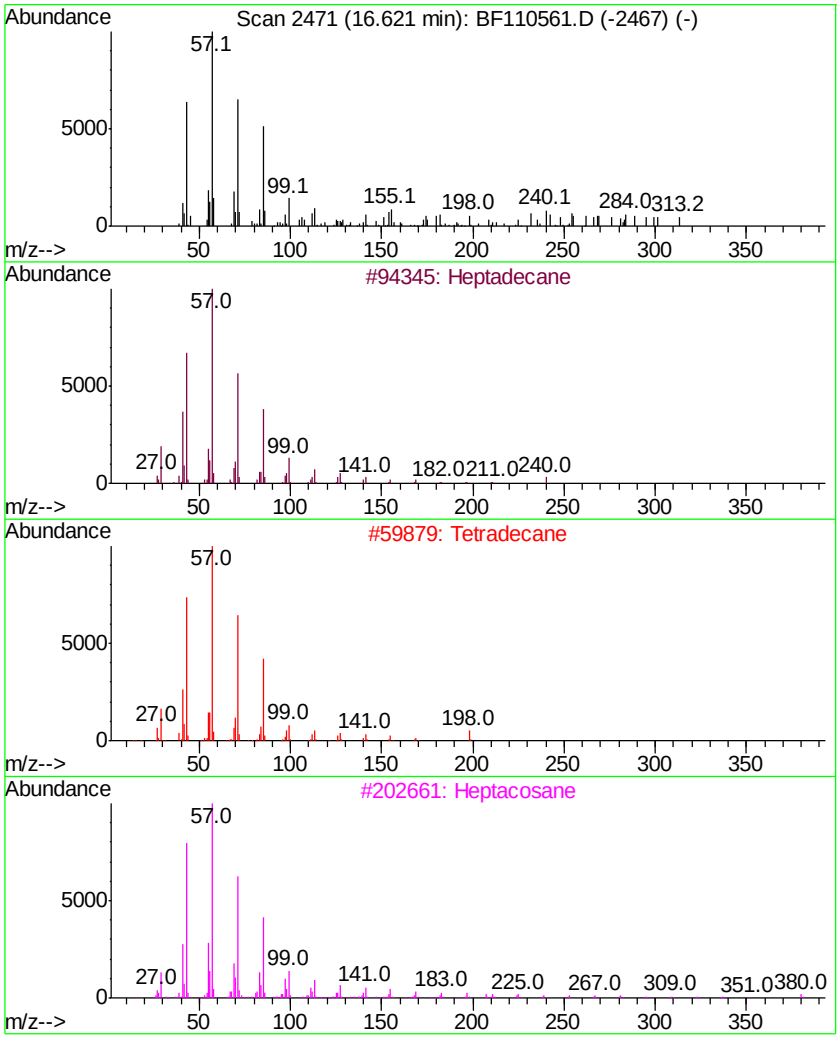
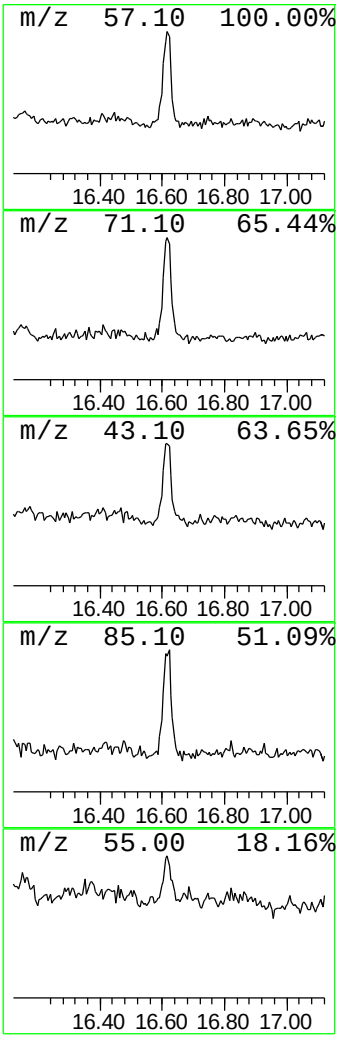
Peak Number 11 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	4.54 ng	92763	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	64
2	Tetradecane	198	C14H30	000629-59-4	58
3	Heptacosane	380	C27H56	000593-49-7	52
4	Docosane	310	C22H46	000629-97-0	52
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110718\
Data File : BF110561.D
Acq On : 7 Nov 2018 17:53
Operator : JU/SJ
Sample : J5762-03 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-110518

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...	2.23	10.4	ng	237605	1	6.95	454547	20.0
unknown6.72	6.72	40.7	ng	924401	1	6.95	454547	20.0
2-Chloroethyl lin...	12.54	2.9	ng	60572	4	11.49	423243	20.0
10-Octadecenoic a...	12.56	5.4	ng	114920	4	11.49	423243	20.0
Heptadecyl heptaf...	13.94	3.3	ng	90593	5	14.13	549371	20.0
Hentriacontane	14.88	6.8	ng	188006	5	14.13	549371	20.0
Tetratetracontane	15.23	8.1	ng	165040	6	15.66	408499	20.0
Pentadecane	16.09	8.4	ng	172439	6	15.66	408499	20.0
Heptadecane	16.62	4.5	ng	92763	6	15.66	408499	20.0