LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110621.D
Acq On : 9 Nov 2018 12:19
Operator : JU/SJ
Sample : J5839-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

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-BF110818.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	2.252	23	28	39	rVB	205870	264443	21.26%	2.405%
2	4.569	419	422	430	rBV	33600	43633	3.51%	0.397%
3	5.169	521	524	535	rBV	50433	64779	5.21%	0.589%
4	5.563	587	591	613	rVB	912556	862783	69.37%	7.846%
5	6.569	758	762	778	rBV	1083425	1154094	92.80%	10.495%
6	6.710	783	786	790	rBV	1248521	1076643	86.57%	9.791%
7	6.945	822	826	832	rBV	512329	435888	35.05%	3.964%
8	7.098	848	852	867	rBV	1011267	884784	71.14%	8.046%
9	7.510	918	922	939	rBV	667742	691547	55.61%	6.289%
10	8.228	1040	1044	1057	rBV	598056	561652	45.16%	5.107%
11	9.298	1222	1226	1242	rVB	1499852	1243672	100.00%	11.310%
12	9.692	1289	1293	1300	rBV	129927	116085	9.33%	1.056%
13	9.986	1339	1343	1351	rBV	599408	538614	43.31%	4.898%
14	10.775	1474	1477	1489	rBV	268569	283105	22.76%	2.574%
15	11.480	1593	1597	1607	rBV	464818	430457	34.61%	3.914%
16	12.769	1813	1816	1820	rBV4	9193	14603	1.17%	0.133%
17	13.063	1862	1866	1869	rVB	938423	853459	68.62%	7.761%
18	13.939	2012	2015	2025	rVB3	33789	61242	4.92%	0.557%
19	14.074	2030	2038	2043	rBV	76929	101623	8.17%	0.924%
20	14.127	2043	2047	2051	rBV	468611	448214	36.04%	4.076%
21	14.257	2067	2069	2073	rVB	26059	20057	1.61%	0.182%
22	14.557	2117	2120	2124	rBV	41364	45174	3.63%	0.411%
23	14.874	2170	2174	2178	rBV3	69352	89724	7.21%	0.816%
24	15.227	2230	2234	2239	rVB	83782	99501	8.00%	0.905%
25	15.621	2297	2301	2303	rBV	80717	102015	8.20%	0.928%
26	15.651	2303	2306	2314	rVB	241930	345820	27.81%	3.145%
27	16.074	2374	2378	2385	rVB	70351	105200	8.46%	0.957%
28	16.604	2463	2468	2473	rBV2	35472	57831	4.65%	0.526%

Sum of corrected areas: 10996642

LSC Report - Integrated Chromatogram

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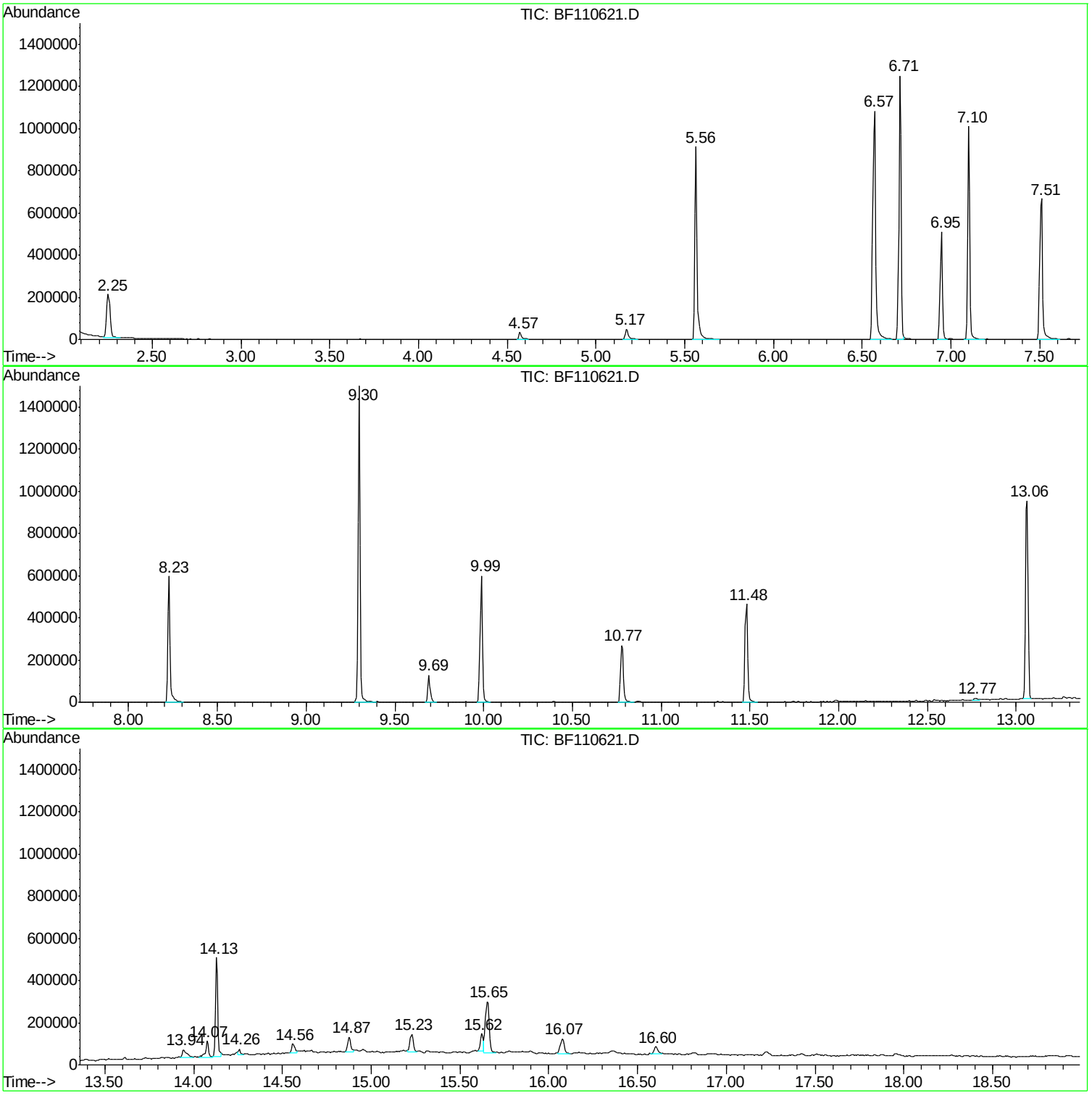
Operator : JU/SJ
Sample : J5839-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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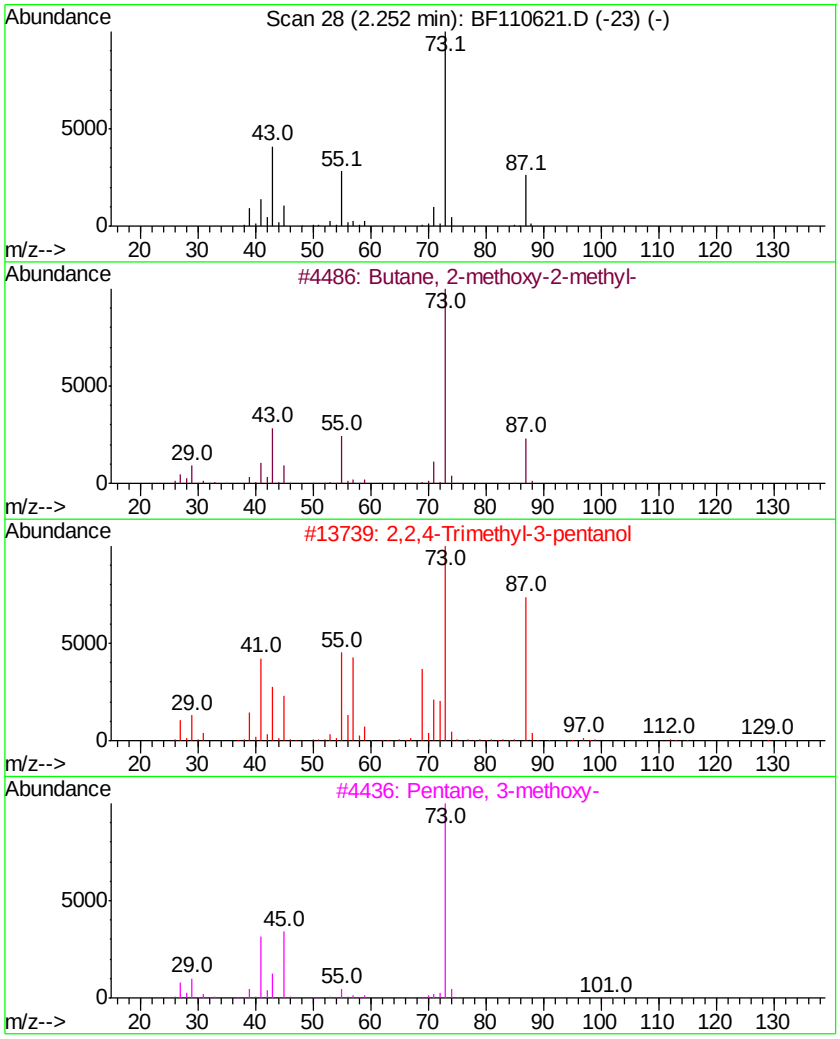
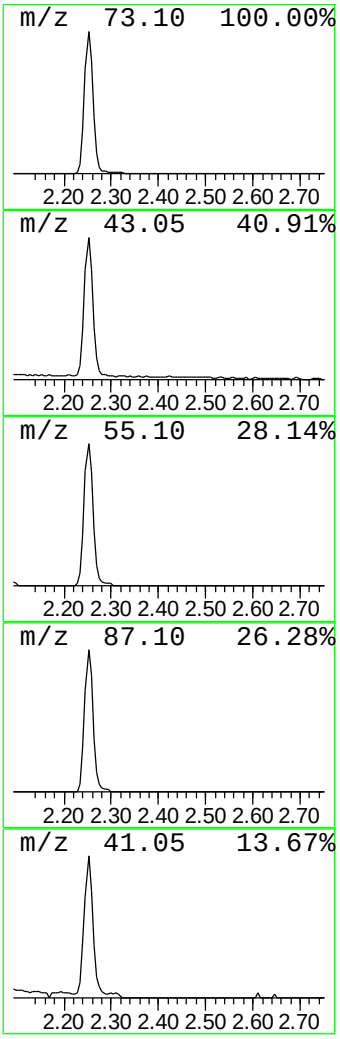
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	12.13 ng	264443	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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Data File : BF110621.D
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Operator : JU/SJ
Sample : J5839-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

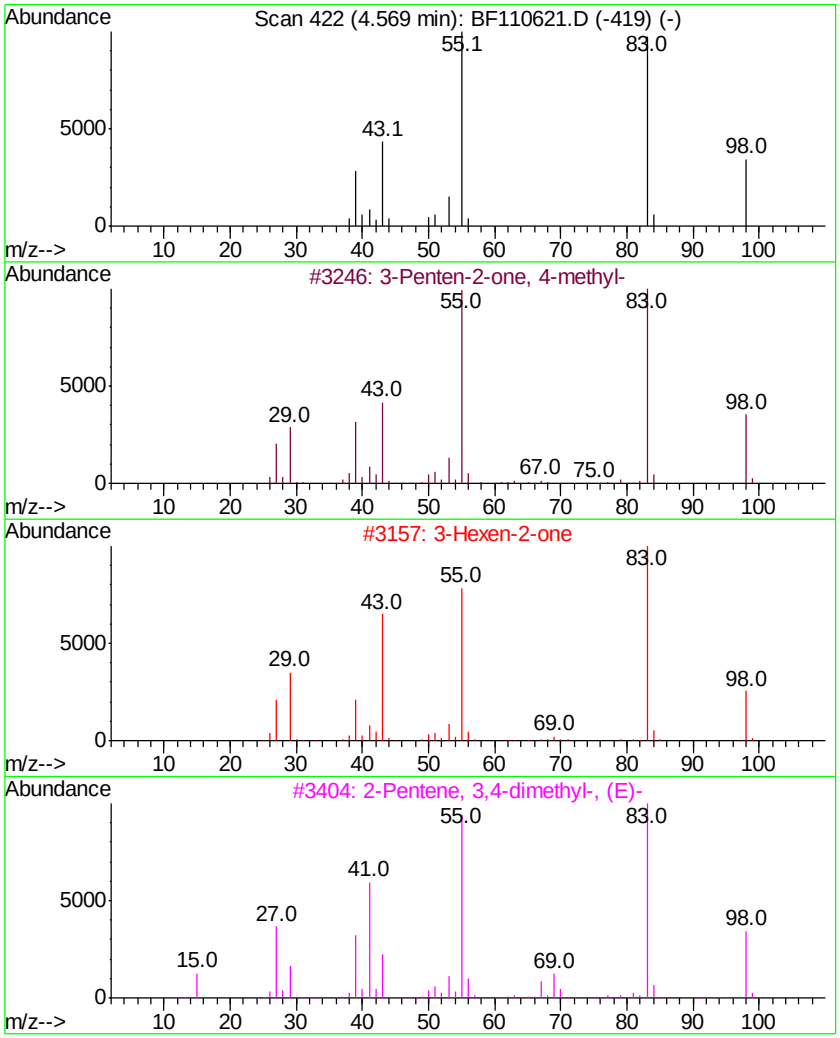
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

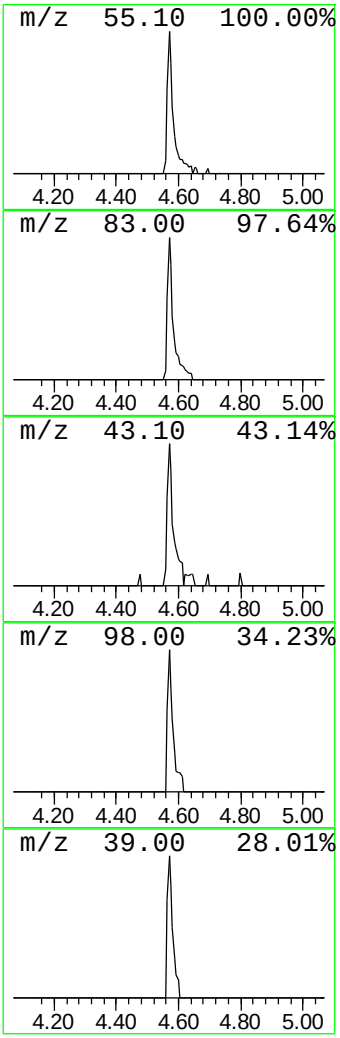
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	2.00 ng	43633	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80





Library Search Compound Report

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Data File : BF110621.D
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Operator : JU/SJ
Sample : J5839-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
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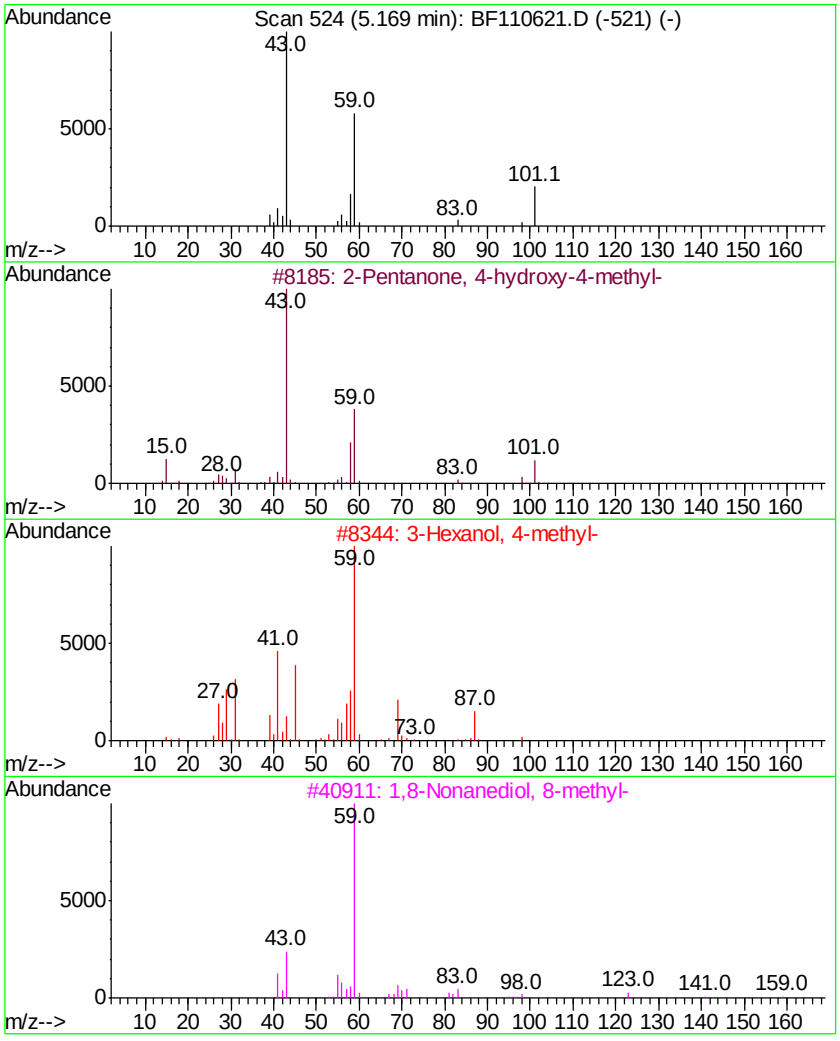
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

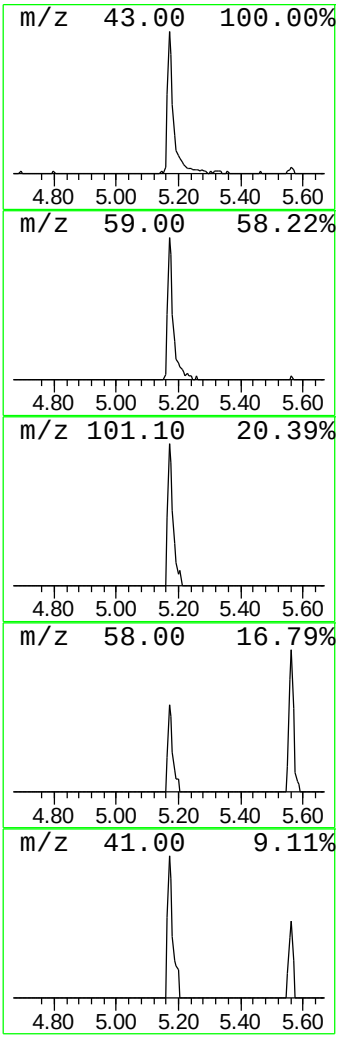
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	2.97 ng	64779	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	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	Acetone	58	C3H6O	000067-64-1	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Library Search Compound Report

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Sample : J5839-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

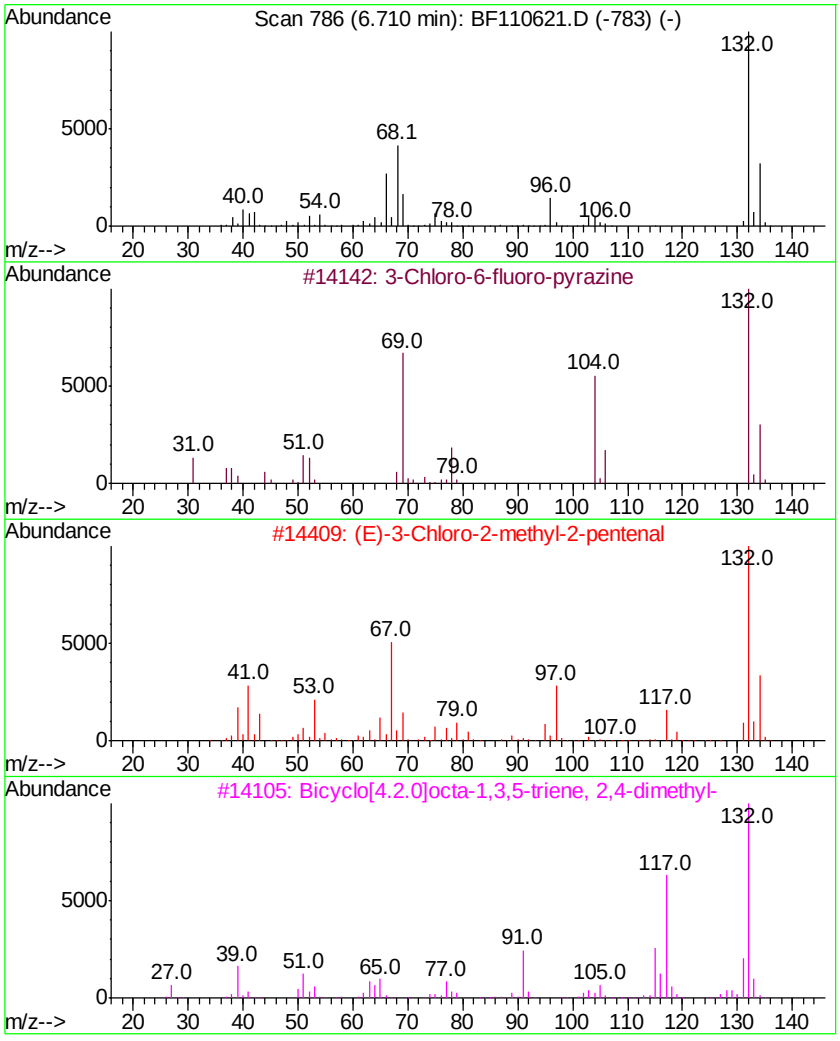
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

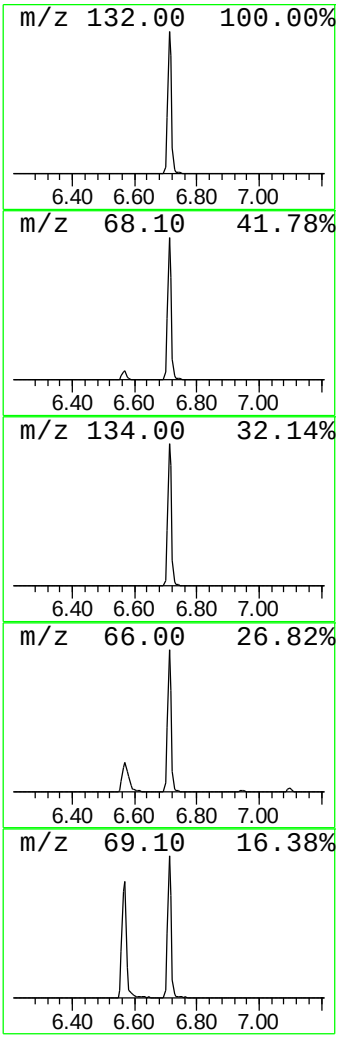
****

Peak Number 4 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	49.40 ng	1076640	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	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Sample : J5839-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

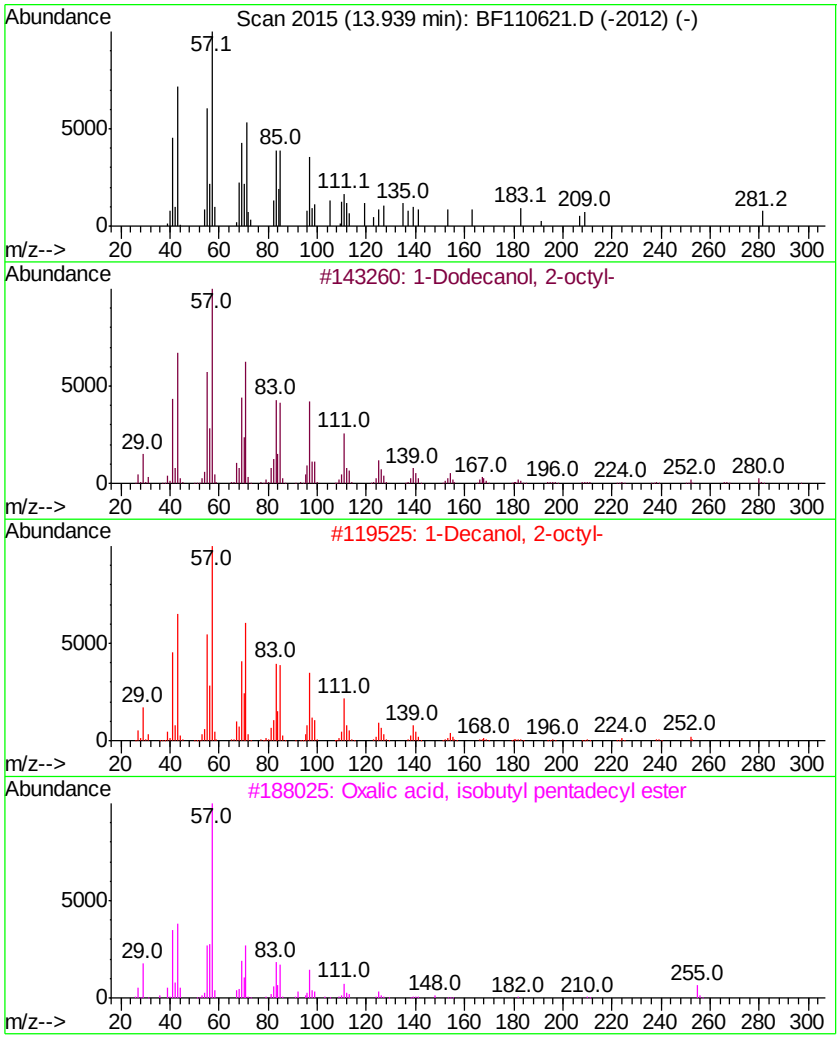
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

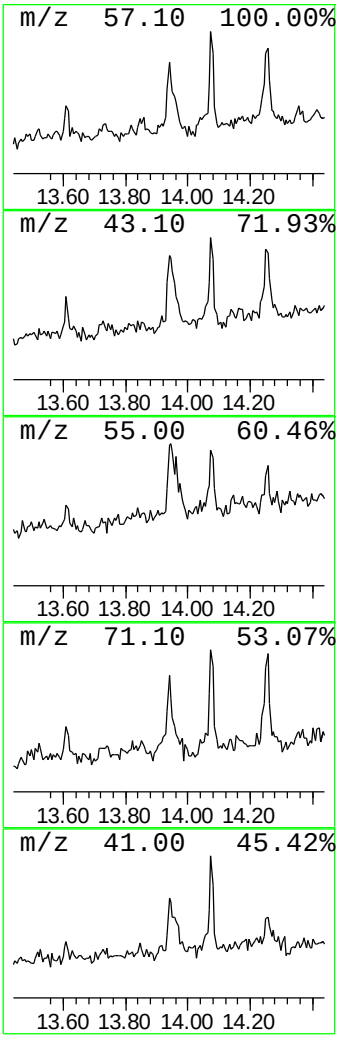
****

Peak Number 6 1-Dodecanol, 2-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.73 ng	61242	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	74
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	68
3	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	64
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	64
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	62





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Sample : J5839-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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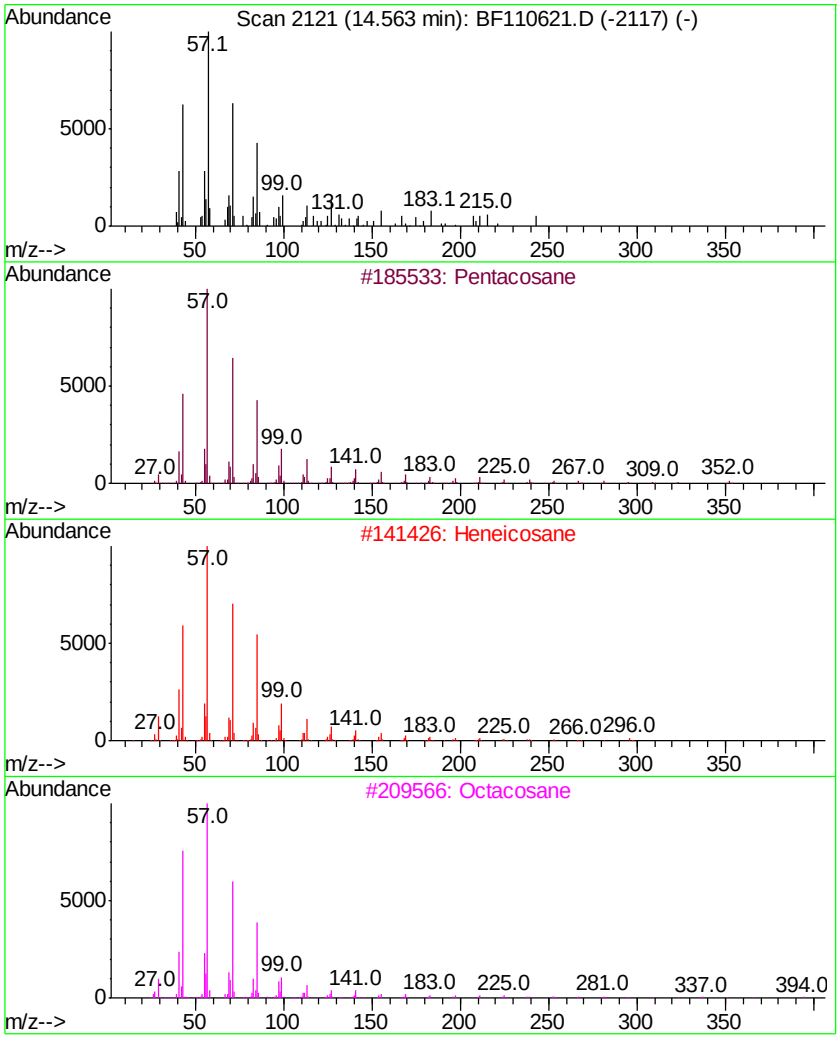
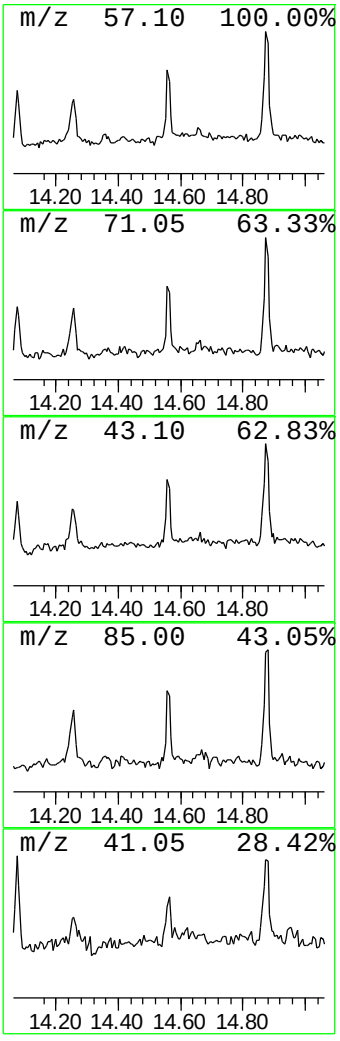
****

Peak Number 7 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.02 ng	45174	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	72
2	Heneicosane	296	C21H44	000629-94-7	72
3	Octacosane	394	C28H58	000630-02-4	68
4	Tetracosane	338	C24H50	000646-31-1	64
5	Heptadecane	240	C17H36	000629-78-7	64





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Sample : J5839-11
Misc :
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Instrument : BNA_F
ClientSampleId : SB-7-S

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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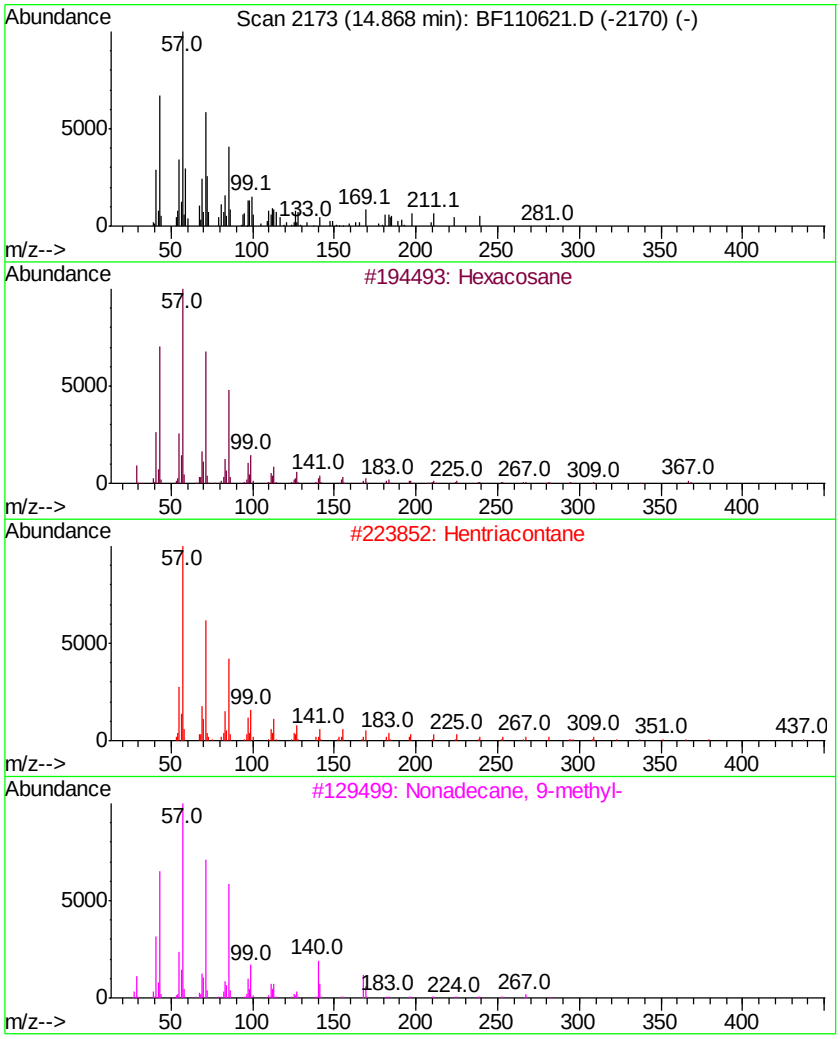
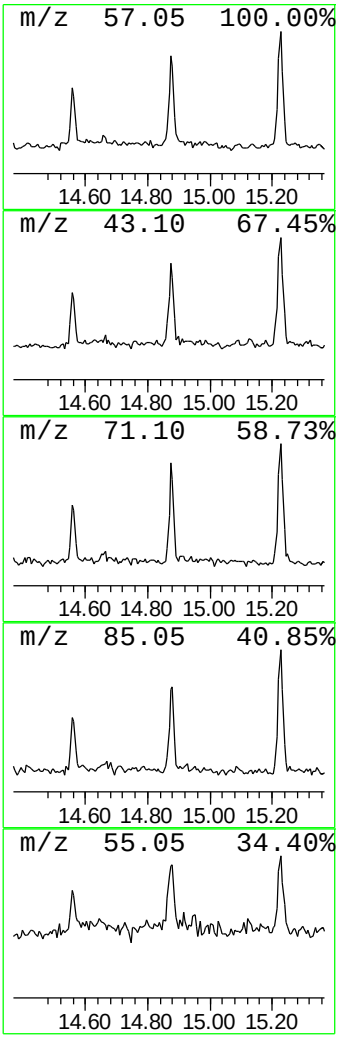
Peak Number 8 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	4.00 ng	89724	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	83
2	Hentriacontane	437	C31H64	000630-04-6	83
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83
4	Heptacosane	380	C27H56	000593-49-7	80
5	Nonadecane	268	C19H40	000629-92-5	72





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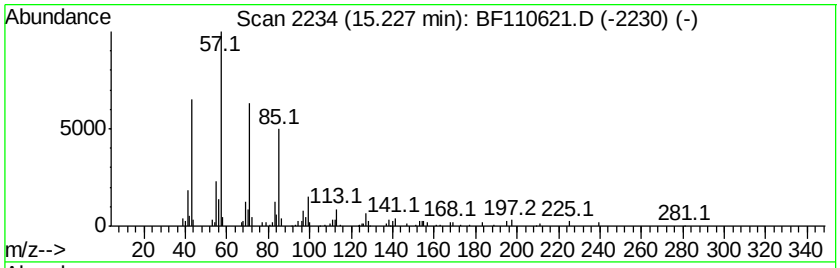
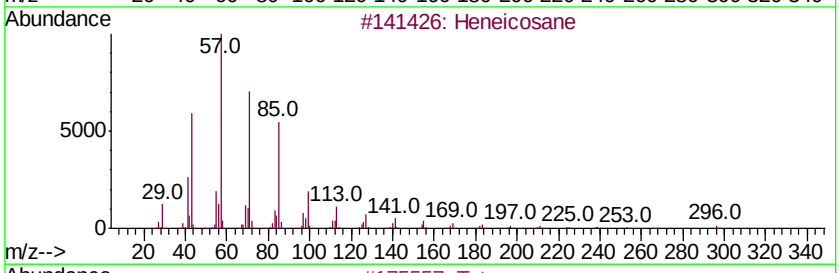
****

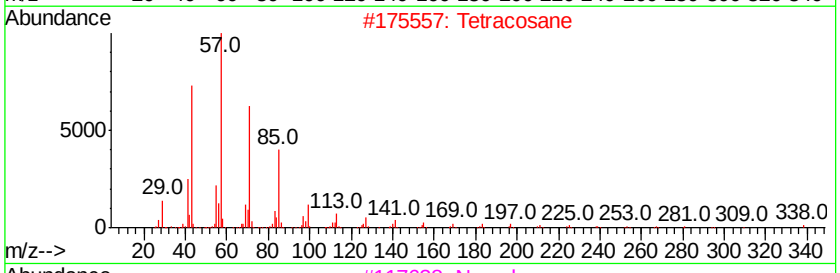
Peak Number 9 Heneicosane Concentration Rank 5

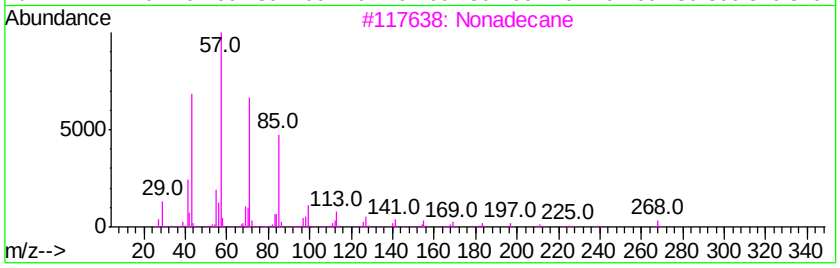
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	5.75 ng	99501	Perylene-d12	15.66

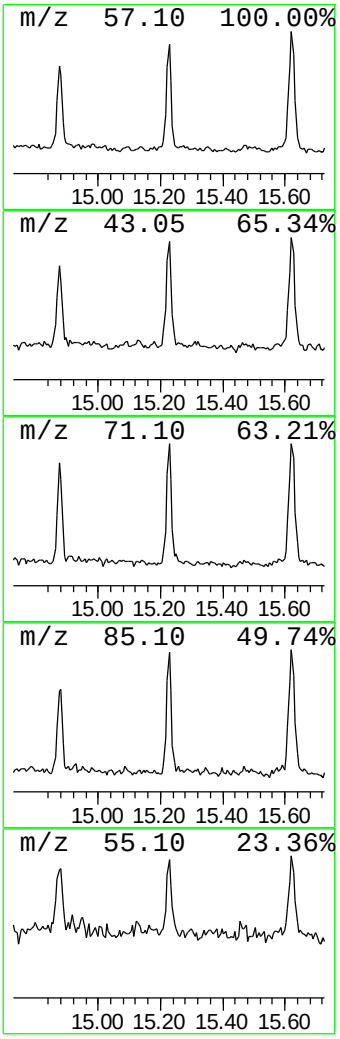
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Nonadecane	268	C19H40	000629-92-5	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Heptadecane	240	C17H36	000629-78-7	91











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Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

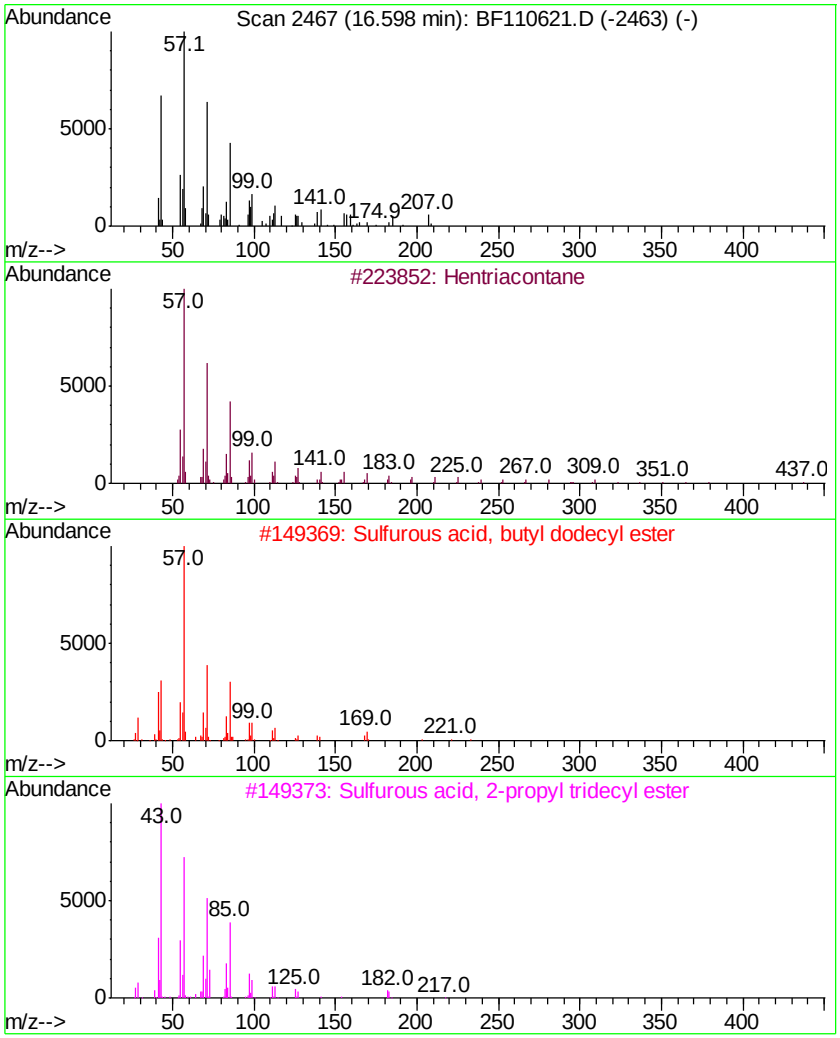
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

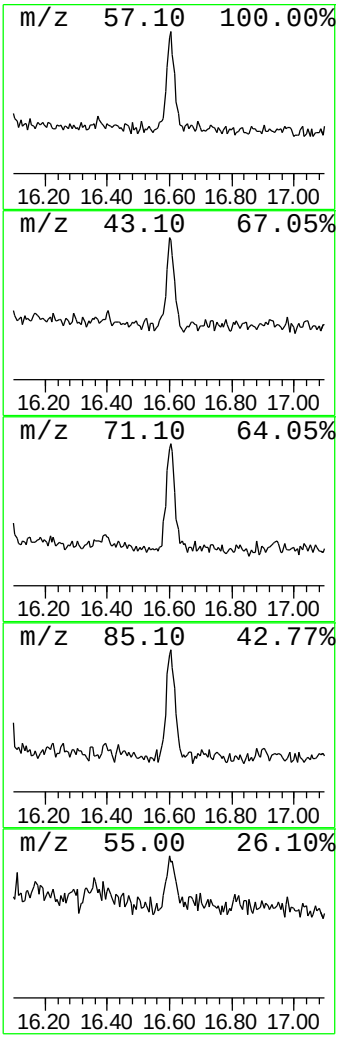
****

Peak Number 11 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	3.34 ng	57831	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	90
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
3	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	72
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	72
5	Tetracosane	338	C24H50	000646-31-1	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
Data File : BF110621.D
Acq On : 9 Nov 2018 12:19
Operator : JU/SJ
Sample : J5839-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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...	2.25	12.1	ng	264443	1	6.95	435888	20.0
3-Penten-2-one, 4...	4.57	2.0	ng	43633	1	6.95	435888	20.0
2-Pentanone, 4-hy...	5.17	3.0	ng	64779	1	6.95	435888	20.0
unknown6.71	6.71	49.4	ng	1076640	1	6.95	435888	20.0
1-Dodecanol, 2-oc...	13.94	2.7	ng	61242	5	14.13	448214	20.0
Pentacosane	14.56	2.0	ng	45174	5	14.13	448214	20.0
Hexacosane	14.87	4.0	ng	89724	5	14.13	448214	20.0
Heneicosane	15.23	5.8	ng	99501	6	15.66	345820	20.0
Hentriacontane	16.60	3.3	ng	57831	6	15.66	345820	20.0