LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108959.D
Acq On : 12 Sep 2018 19:26
Operator : JU/SJ
Sample : J4856-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

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-BF090518.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	4.284	327	331	340	rBV	91454	117109	5.15%	0.511%
2	4.925	436	440	450	rVB	163597	192681	8.48%	0.841%
3	5.342	507	511	515	rBV	1863031	1722498	75.82%	7.515%
4	6.366	680	685	688	rBV	2137311	1832599	80.66%	7.995%
5	6.501	704	708	711	rBV	2208768	1874970	82.53%	8.180%
6	6.736	744	748	751	rBV	1225933	943894	41.55%	4.118%
7	6.889	770	774	778	rBV	1726875	1545866	68.04%	6.744%
8	7.289	838	842	846	rBV	1323305	1191754	52.45%	5.199%
9	8.019	962	966	969	rBV	1374050	1211429	53.32%	5.285%
10	9.089	1144	1148	1152	rBV	2610784	2271975	100.00%	9.912%
11	9.483	1211	1215	1222	rBV	548863	437504	19.26%	1.909%
12	9.766	1259	1263	1275	rBV2	1545662	1346613	59.27%	5.875%
13	10.548	1392	1396	1410	rBV	1208219	1086190	47.81%	4.739%
14	11.242	1510	1514	1517	rBV	1502162	1224487	53.90%	5.342%
15	11.777	1603	1605	1609	rBV3	26756	26806	1.18%	0.117%
16	12.824	1779	1783	1786	rBV	1848072	1653899	72.80%	7.216%
17	13.071	1820	1825	1829	rBV	26013	28366	1.25%	0.124%
18	13.412	1880	1883	1888	rVB	30112	26804	1.18%	0.117%
19	13.742	1932	1939	1952	rBV	121937	247420	10.89%	1.079%
20	13.865	1956	1960	1964	rBV	1872434	1570670	69.13%	6.852%
21	14.054	1988	1992	1999	rBV	59201	60603	2.67%	0.264%
22	14.354	2040	2043	2046	rBV	84847	84605	3.72%	0.369%
23	14.654	2090	2094	2099	rVB	131653	133414	5.87%	0.582%
24	14.724	2102	2106	2110	rBV2	41445	44469	1.96%	0.194%
25	14.971	2144	2148	2152	rVB	170775	169923	7.48%	0.741%
26	15.271	2194	2199	2204	rBV	908208	1127285	49.62%	4.918%
27	15.330	2204	2209	2214	rVB	162318	212039	9.33%	0.925%
28	15.736	2272	2278	2283	rBV	146139	221012	9.73%	0.964%
29	16.200	2352	2357	2367	rVB	103191	177514	7.81%	0.774%
30	16.753	2446	2451	2459	rVB2	44285	88528	3.90%	0.386%
31	17.400	2557	2561	2568	rVB4	24544	48331	2.13%	0.211%

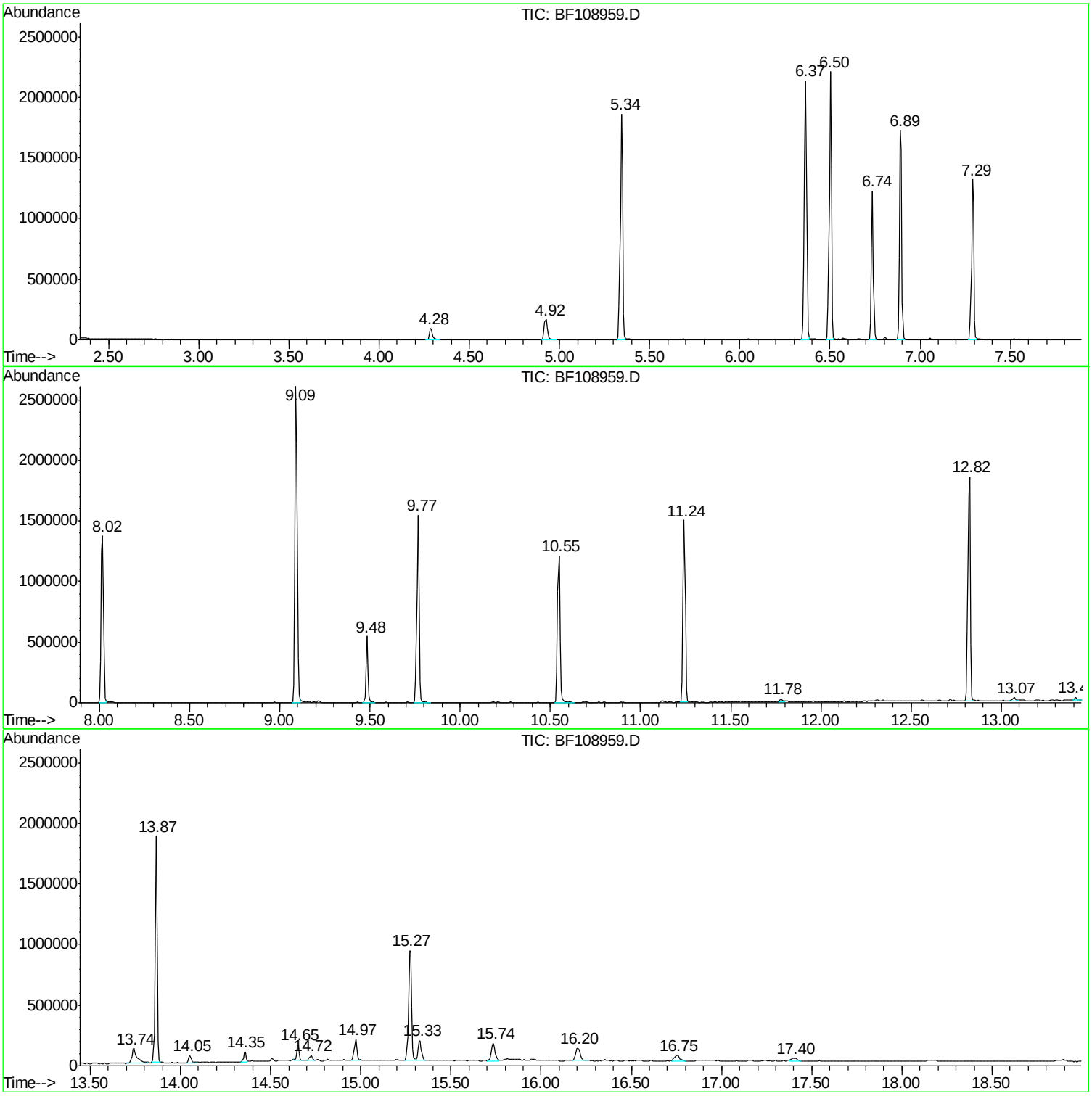
Sum of corrected areas: 22921257

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108959.D
Acq On : 12 Sep 2018 19:26
Operator : JU/SJ
Sample : J4856-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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\BF091218\
Data File : BF108959.D
Acq On : 12 Sep 2018 19:26
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Sample : J4856-05
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

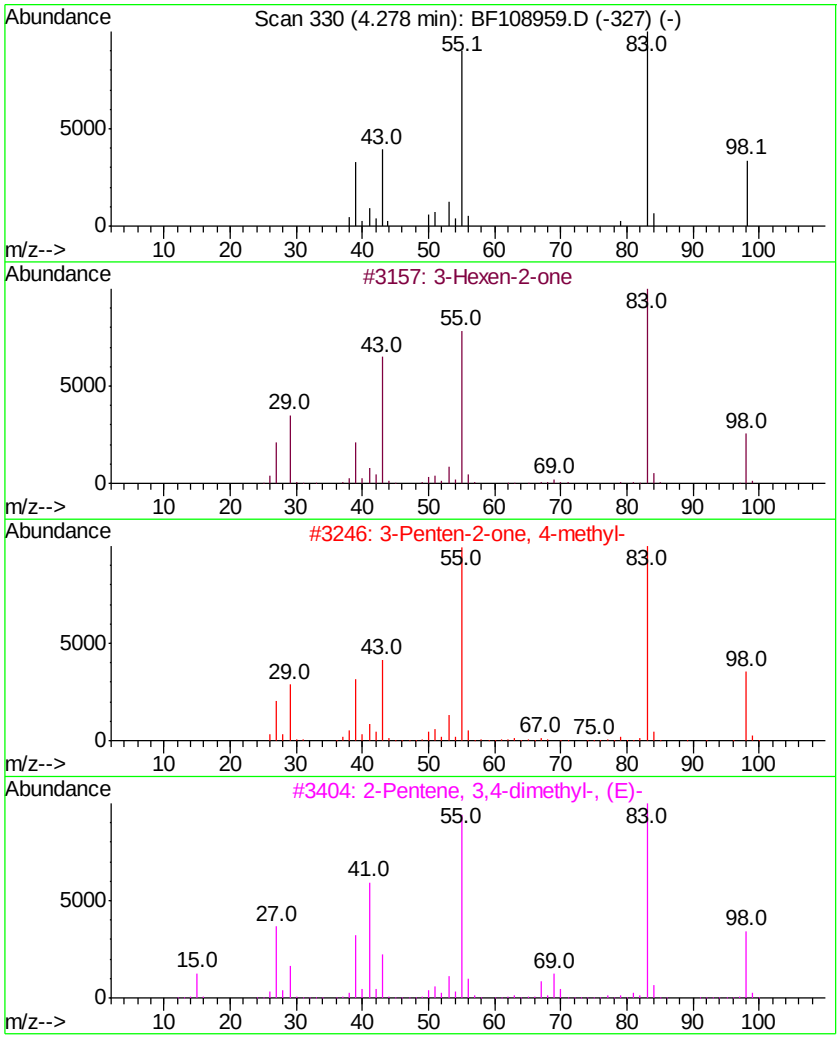
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

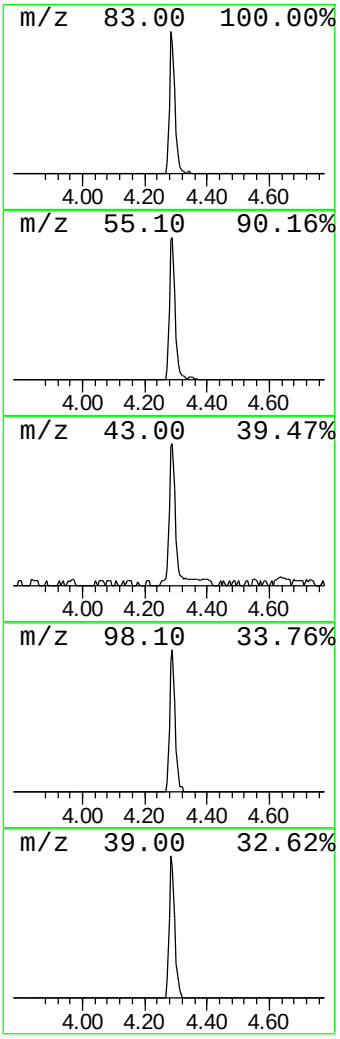
****

Peak Number 1 3-Hexen-2-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	2.48 ng	117109	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108959.D
Acq On : 12 Sep 2018 19:26
Operator : JU/SJ
Sample : J4856-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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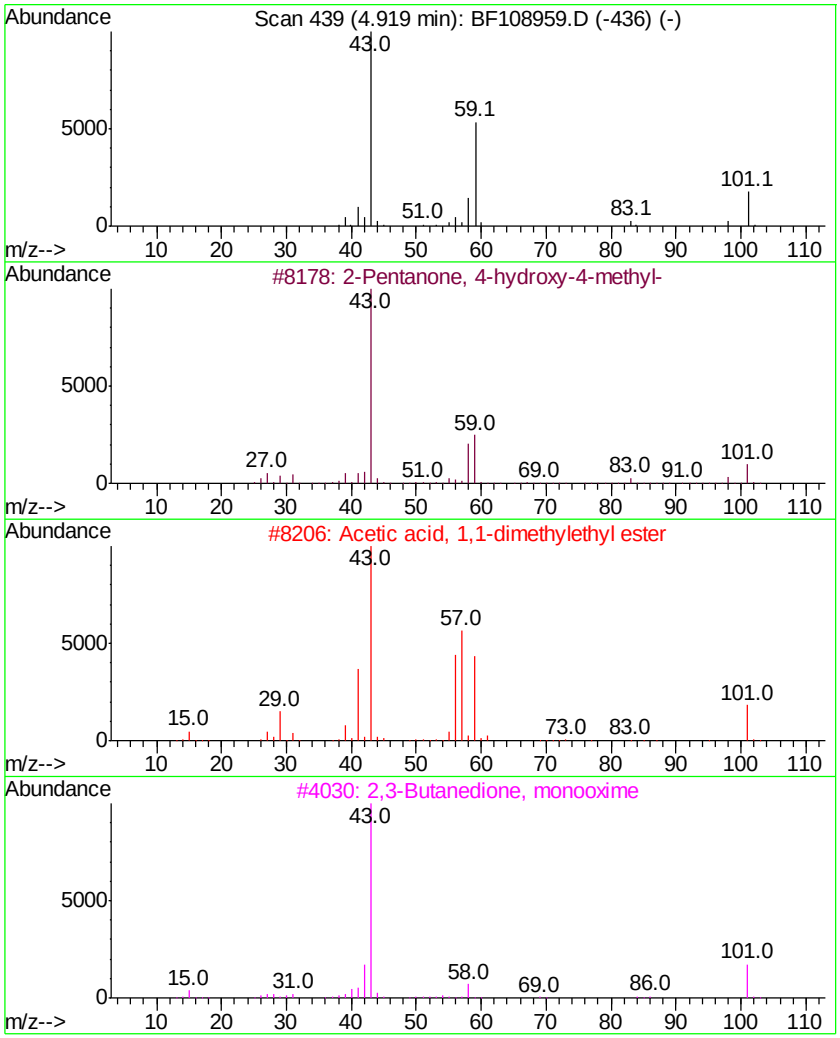
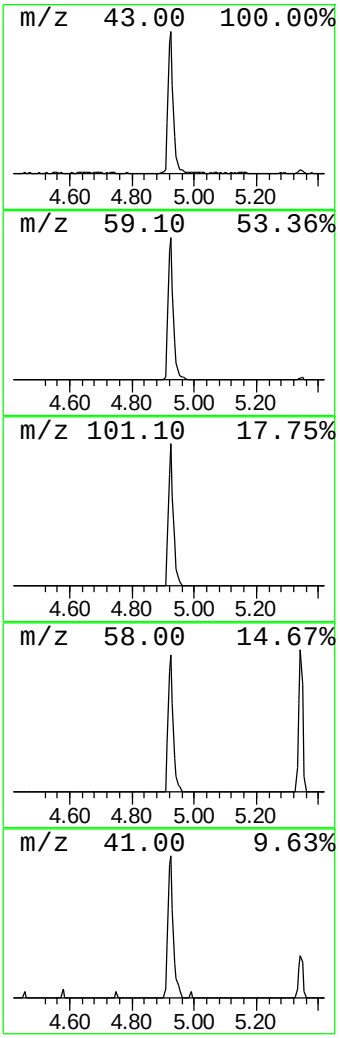
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	4.08 ng	192681	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108959.D
Acq On : 12 Sep 2018 19:26
Operator : JU/SJ
Sample : J4856-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

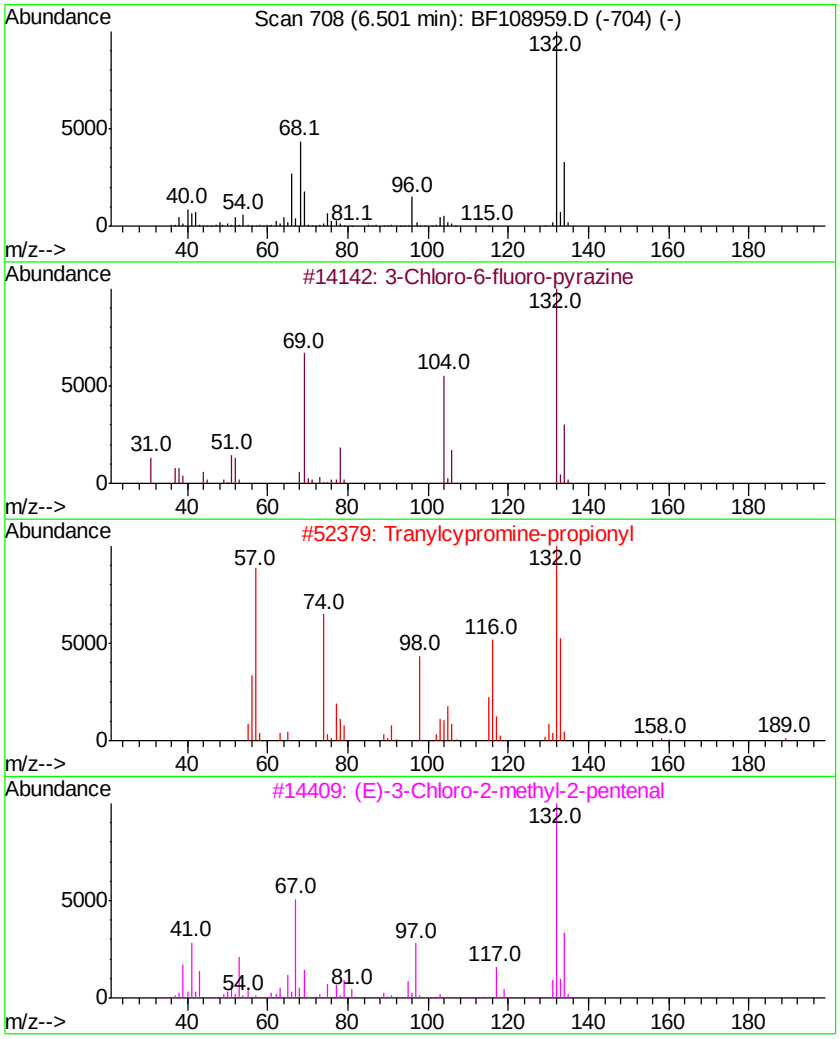
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

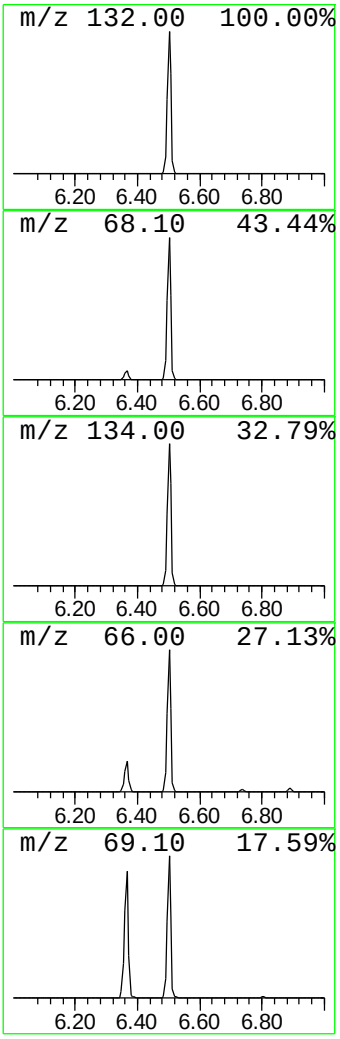
****

Peak Number 3 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	39.73 ng	1874970	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108959.D
Acq On : 12 Sep 2018 19:26
Operator : JU/SJ
Sample : J4856-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

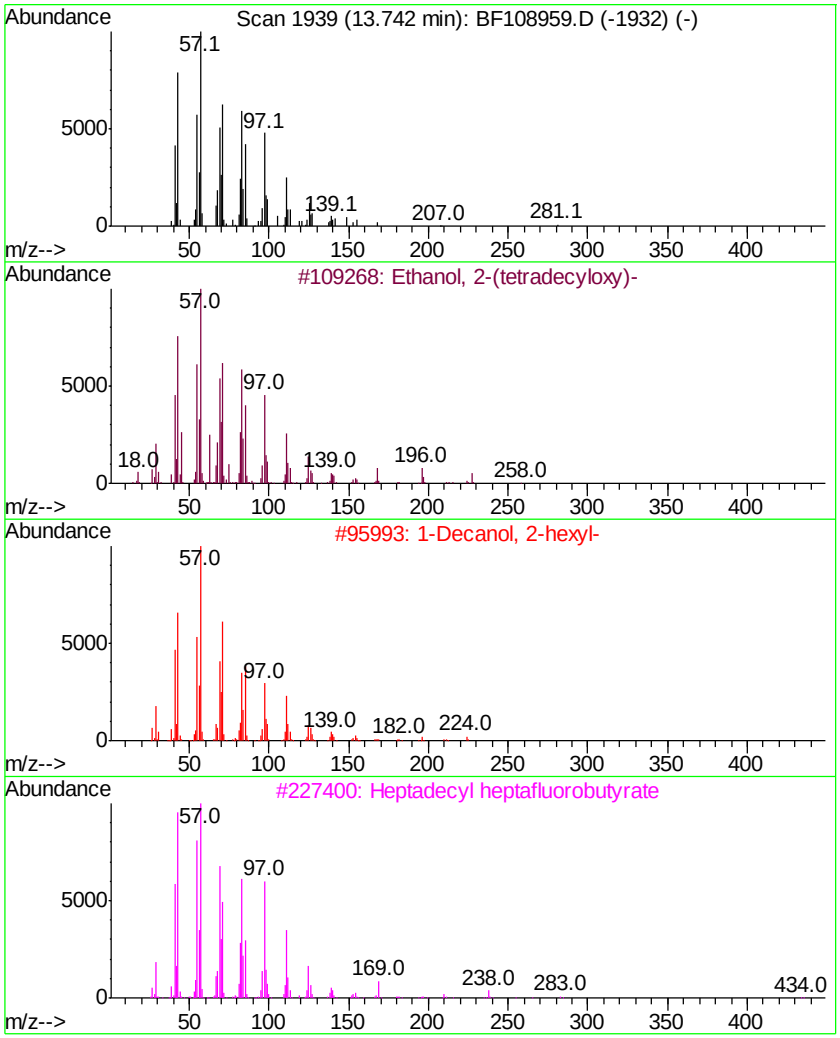
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

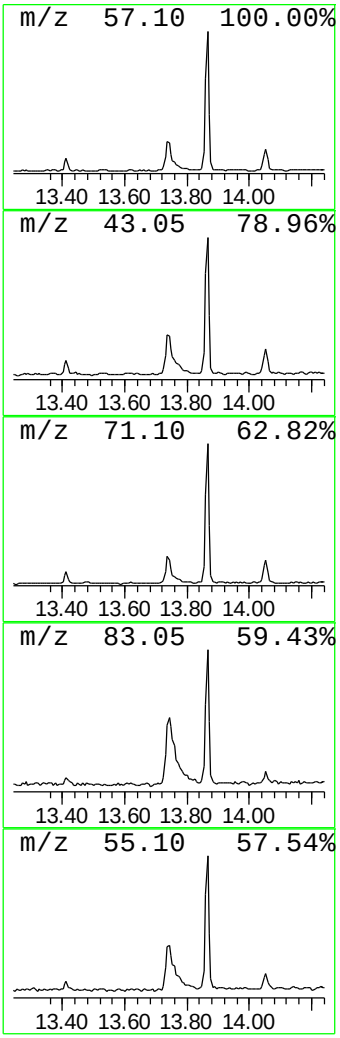
****

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.15 ng	247420	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	81
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	76
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108959.D
Acq On : 12 Sep 2018 19:26
Operator : JU/SJ
Sample : J4856-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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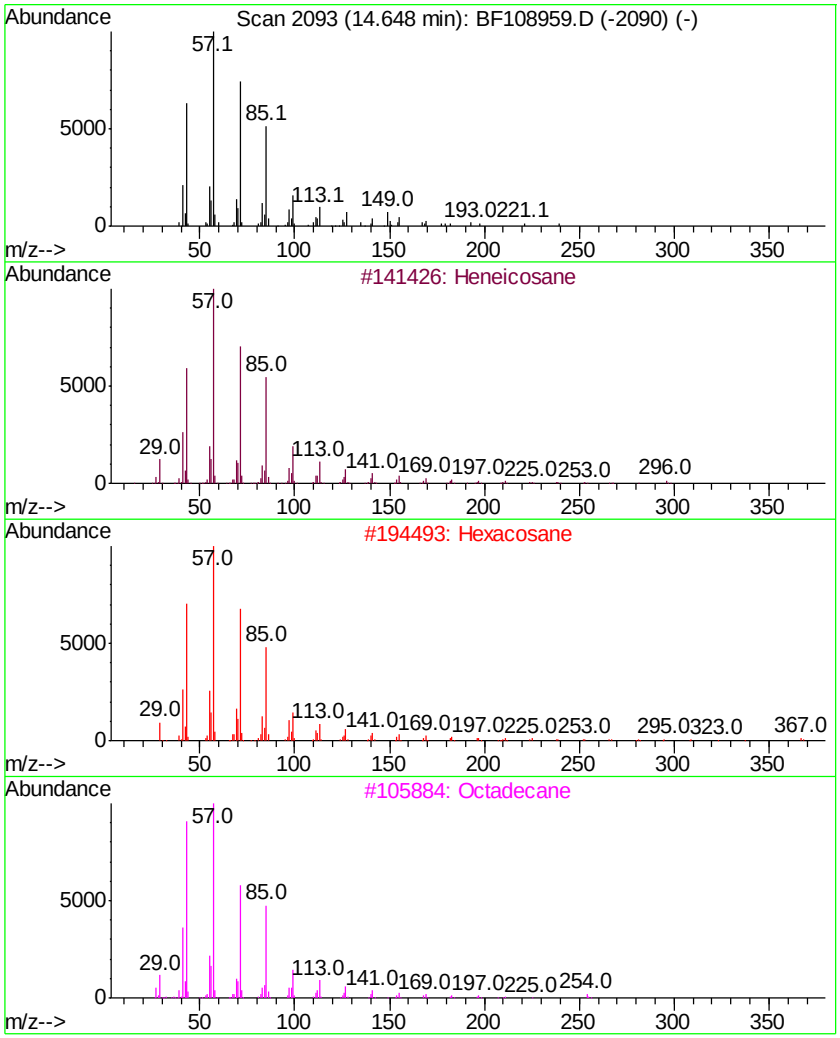
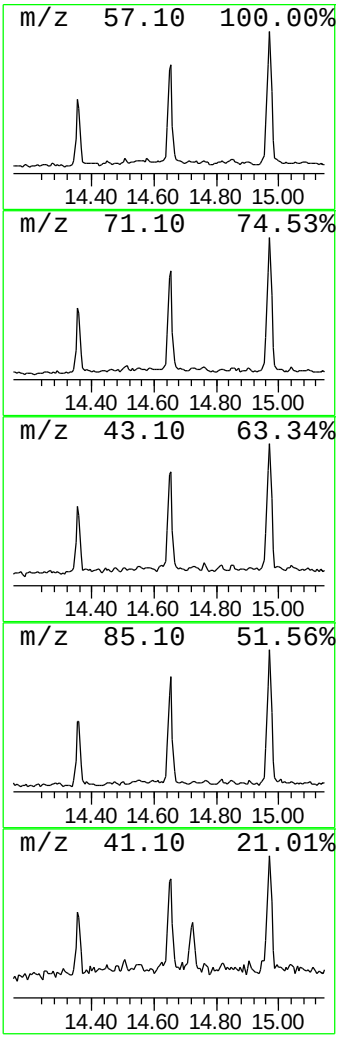
Peak Number 6 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.37 ng	133414	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Docosane	310	C22H46	000629-97-0	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





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Misc :
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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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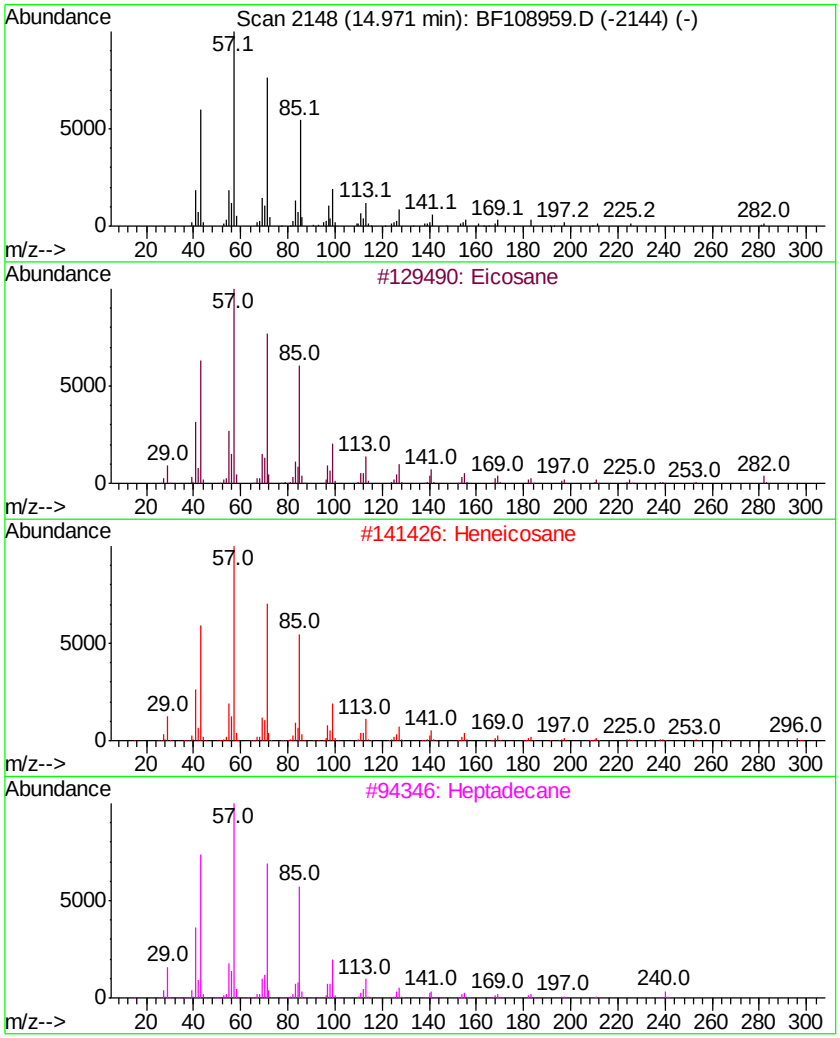
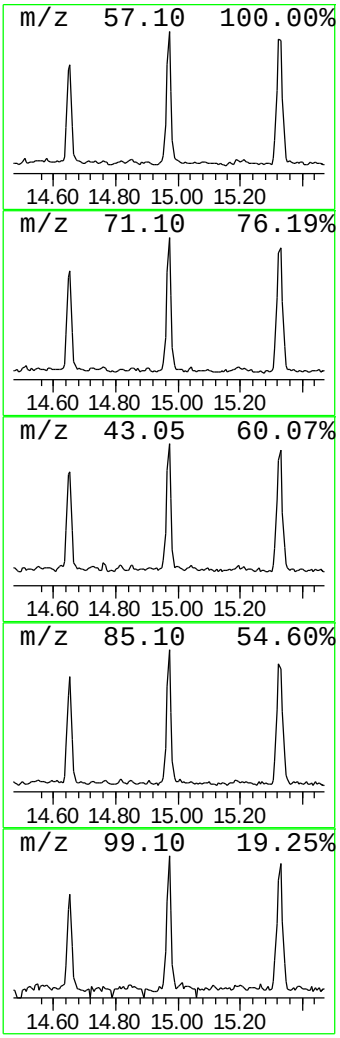
Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	3.01 ng	169923	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
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Operator : JU/SJ
Sample : J4856-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

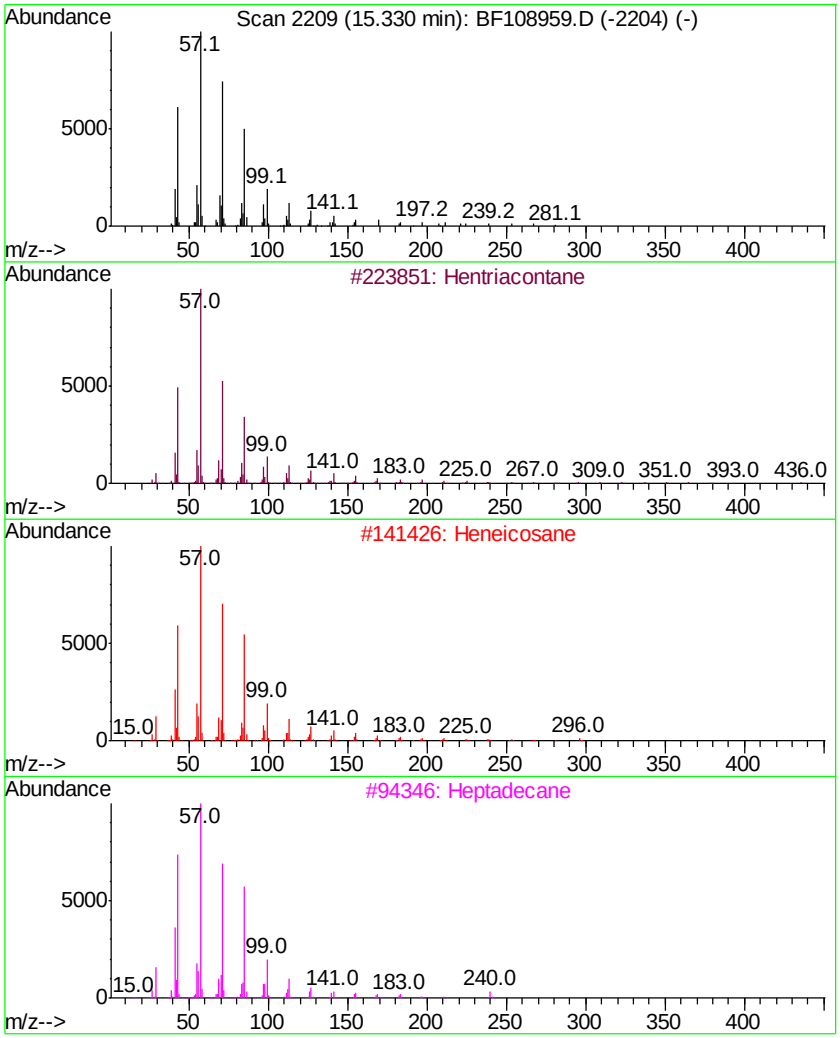
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

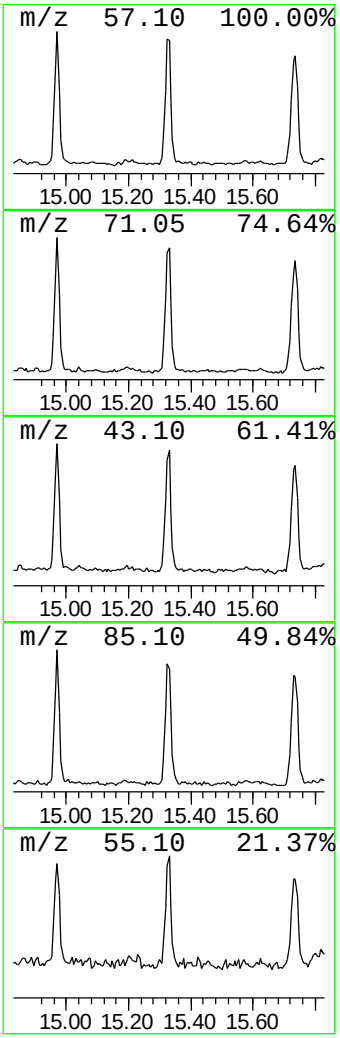
****

Peak Number 8 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	3.76 ng	212039	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexacosane	366	C26H54	000630-01-3	90





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Sample : J4856-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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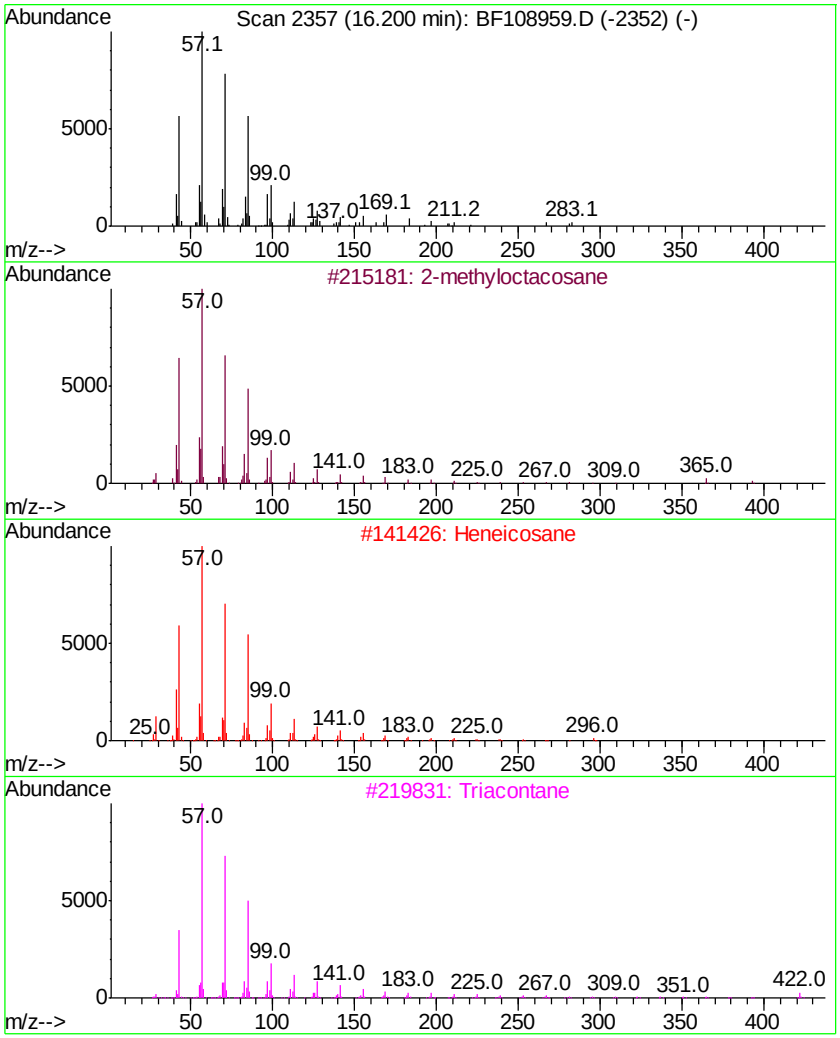
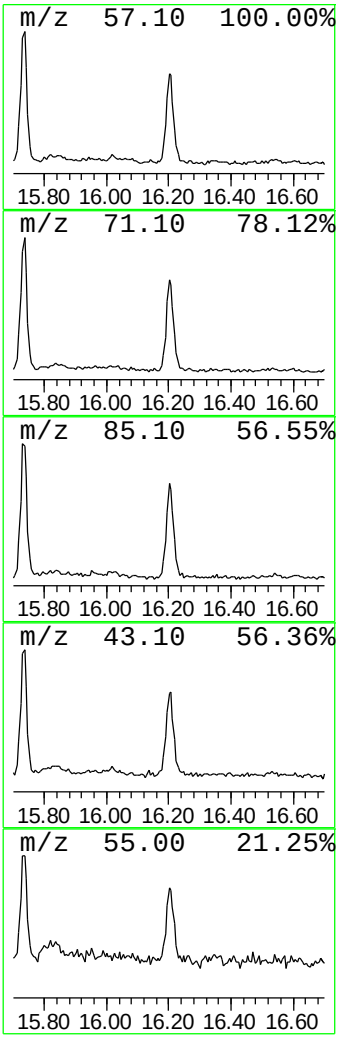
Peak Number 10 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	3.15 ng	177514	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Triacontane	422	C30H62	000638-68-6	90
4	Octadecane	254	C18H38	000593-45-3	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091218\
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Operator : JU/SJ
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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
3-Hexen-2-one	4.28	2.5	ng	117109	1	6.74	943894	20.0
2-Pentanone, 4-hy...	4.92	4.1	ng	192681	1	6.74	943894	20.0
unknown6.50	6.50	39.7	ng	1874970	1	6.74	943894	20.0
Ethanol, 2-(tetra...	13.74	3.1	ng	247420	5	13.87	1570670	20.0
Heneicosane	14.65	2.4	ng	133414	6	15.27	1127290	20.0
Eicosane	14.97	3.0	ng	169923	6	15.27	1127290	20.0
Hentriacontane	15.33	3.8	ng	212039	6	15.27	1127290	20.0
2-methyloctacosane	16.20	3.1	ng	177514	6	15.27	1127290	20.0