LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117559.D
Acq On : 28 Oct 2019 14:16
Operator : JU
Sample : K5501-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 186-14-(0-2.1)

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-BF101819.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	5.351	552	555	576	rBV	715720	860089	78.91%	9.773%
2	6.381	726	730	747	rBV	878569	960678	88.14%	10.916%
3	6.504	747	751	764	rVB	1011615	988020	90.65%	11.227%
4	6.728	786	789	799	rVB	229248	221763	20.35%	2.520%
5	6.881	811	815	828	rBV	822386	731070	67.08%	8.307%
6	7.292	881	885	903	rBV	528560	579211	53.14%	6.581%
7	8.010	1003	1007	1023	rBV	244906	286725	26.31%	3.258%
8	9.081	1185	1189	1202	rBV	1264069	1089900	100.00%	12.384%
9	9.481	1253	1257	1270	rBB	98611	98910	9.08%	1.124%
10	9.757	1301	1304	1316	rBV	361744	336297	30.86%	3.821%
11	10.551	1436	1439	1453	rBV	546608	575722	52.82%	6.542%
12	11.245	1554	1557	1566	rBV	316629	323424	29.67%	3.675%
13	11.775	1644	1647	1661	rBV2	29731	35549	3.26%	0.404%
14	12.698	1798	1804	1810	rBV	14918	16525	1.52%	0.188%
15	12.827	1822	1826	1829	rBV	1101963	968204	88.83%	11.001%
16	13.727	1974	1979	1987	rBV3	42183	70833	6.50%	0.805%
17	13.892	2003	2007	2018	rBV	217545	230258	21.13%	2.616%
18	14.039	2026	2032	2035	rBV	13572	12989	1.19%	0.148%
19	14.345	2080	2084	2087	rBV	21846	21406	1.96%	0.243%
20	14.639	2131	2134	2138	rBV	36263	33641	3.09%	0.382%
21	14.710	2143	2146	2149	rVB	38526	33150	3.04%	0.377%
22	14.957	2184	2188	2193	rVB	39144	42680	3.92%	0.485%
23	15.327	2244	2251	2259	rVB	153906	236265	21.68%	2.685%
24	15.715	2313	2317	2322	rVB2	21670	29657	2.72%	0.337%
25	16.180	2392	2396	2400	rBV4	15301	17794	1.63%	0.202%

Sum of corrected areas: 8800760

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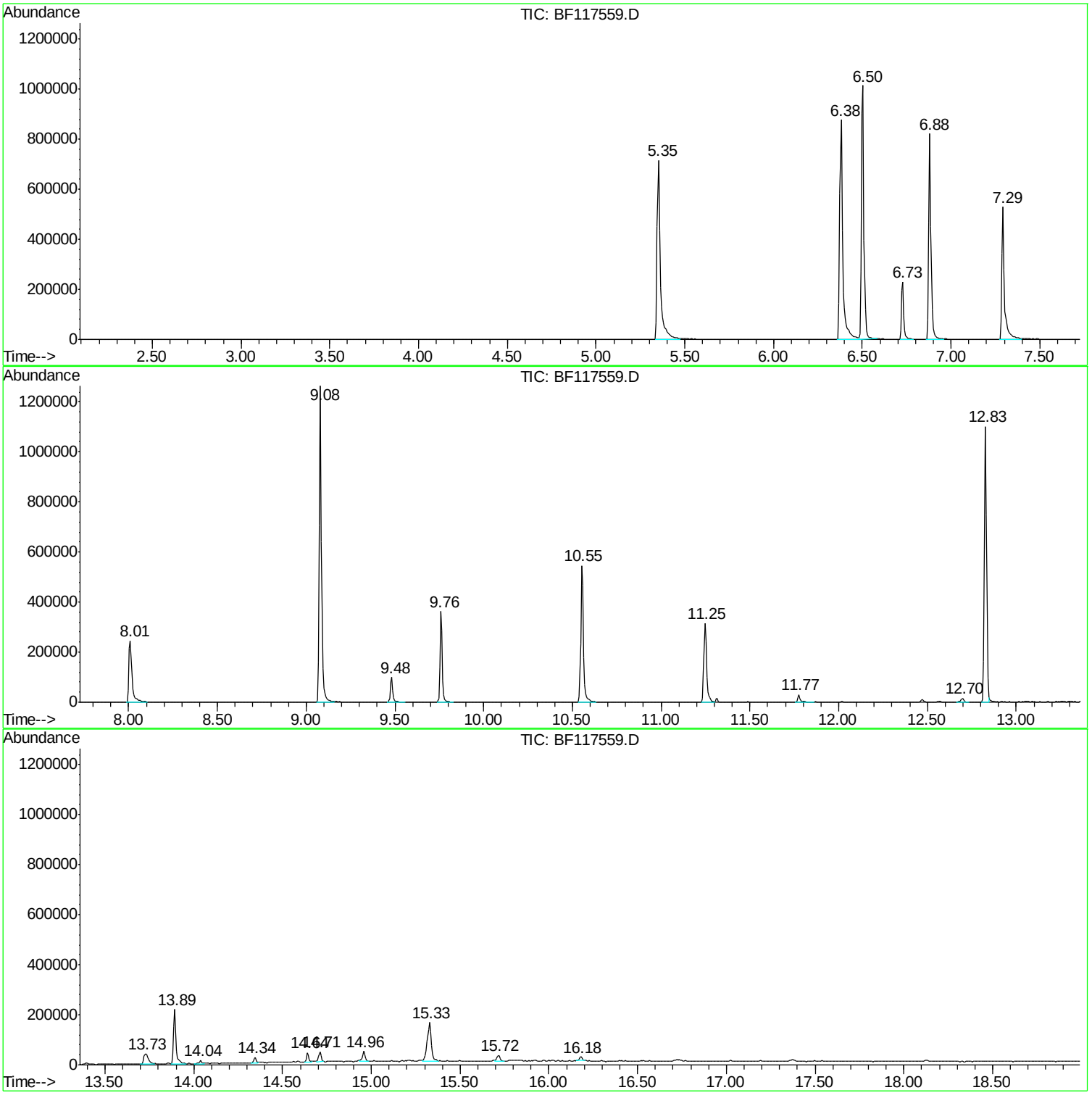
Instrument :
BNA_F
ClientSampleId :
186-14-(0-2.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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ClientSampleId : 186-14-(0-2.1)

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TIC Library : C:\DATABASE\NIST11.L
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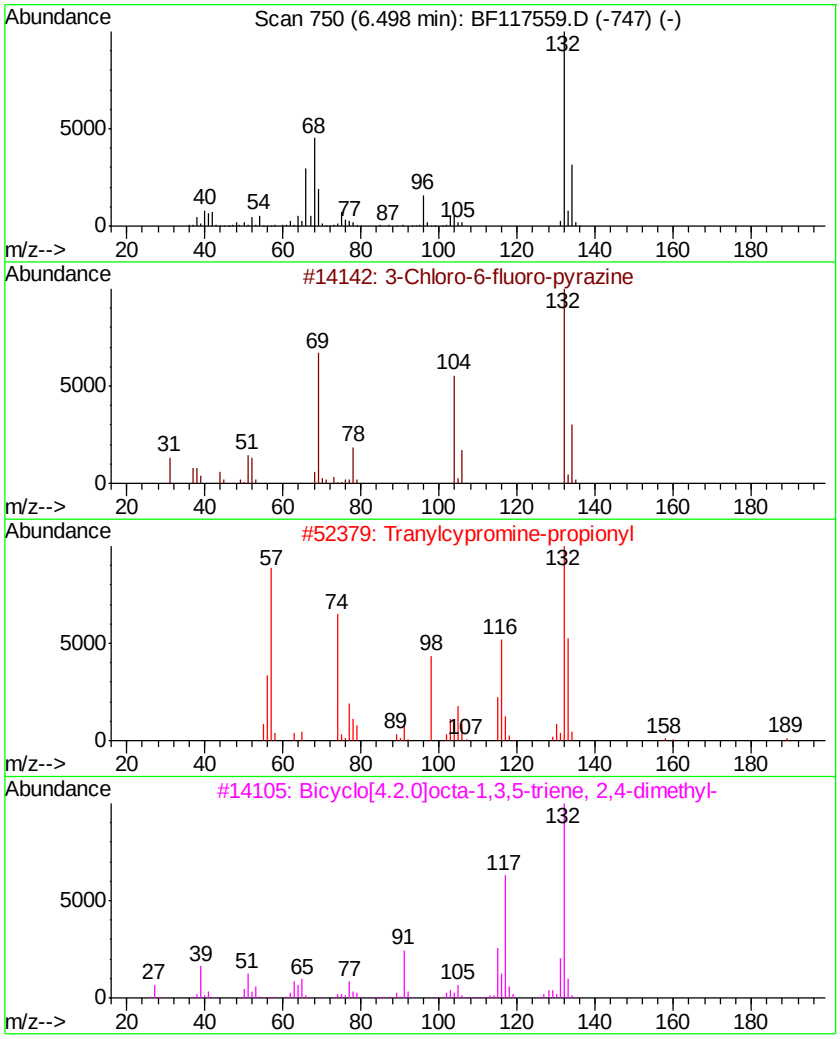
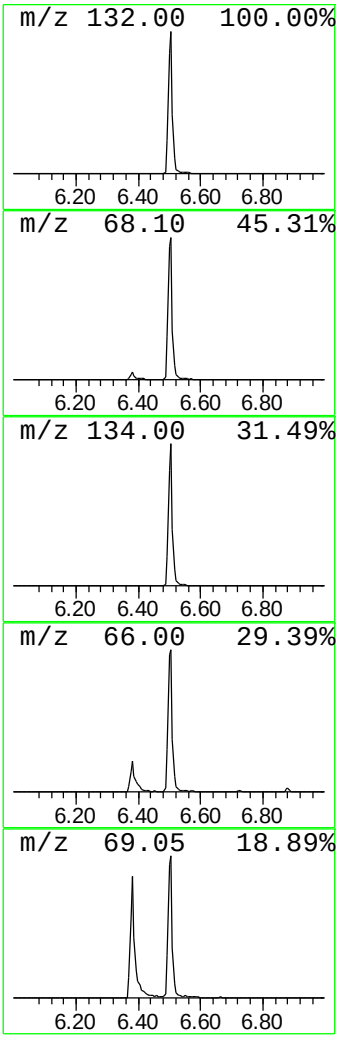
Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	89.11 ng	988020	1,4-Dichlorobenzene-d4	6.73

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	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Misc :
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Instrument : BNA_F
ClientSampleId : 186-14-(0-2.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
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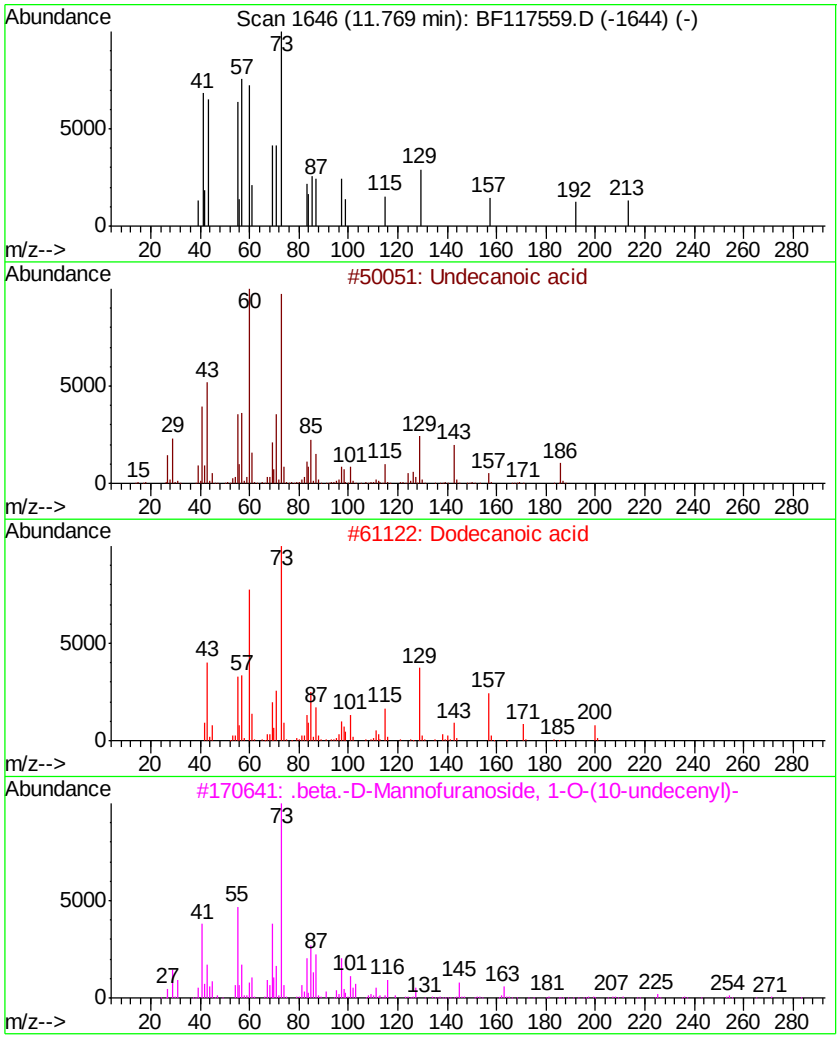
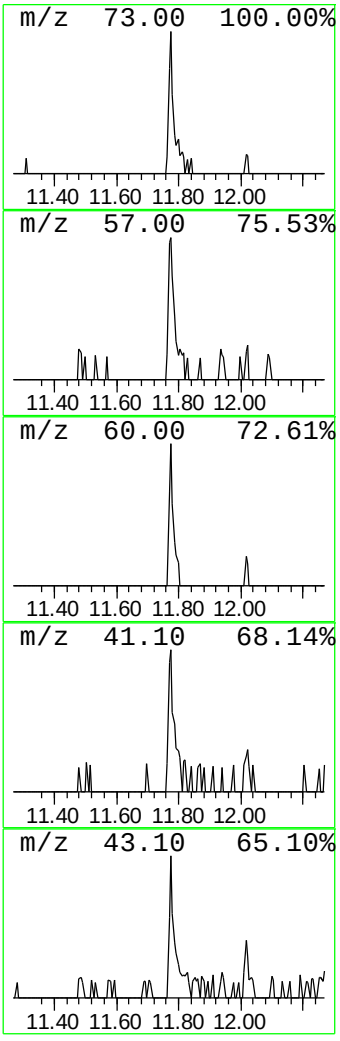
Peak Number 3 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.20 ng	35549	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	64
2	Dodecanoic acid	200	C12H24O2	000143-07-7	59
3	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	18
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	18





Library Search Compound Report

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Operator : JU
Sample : K5501-07
Misc :
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Instrument : BNA_F
ClientSampleId : 186-14-(0-2.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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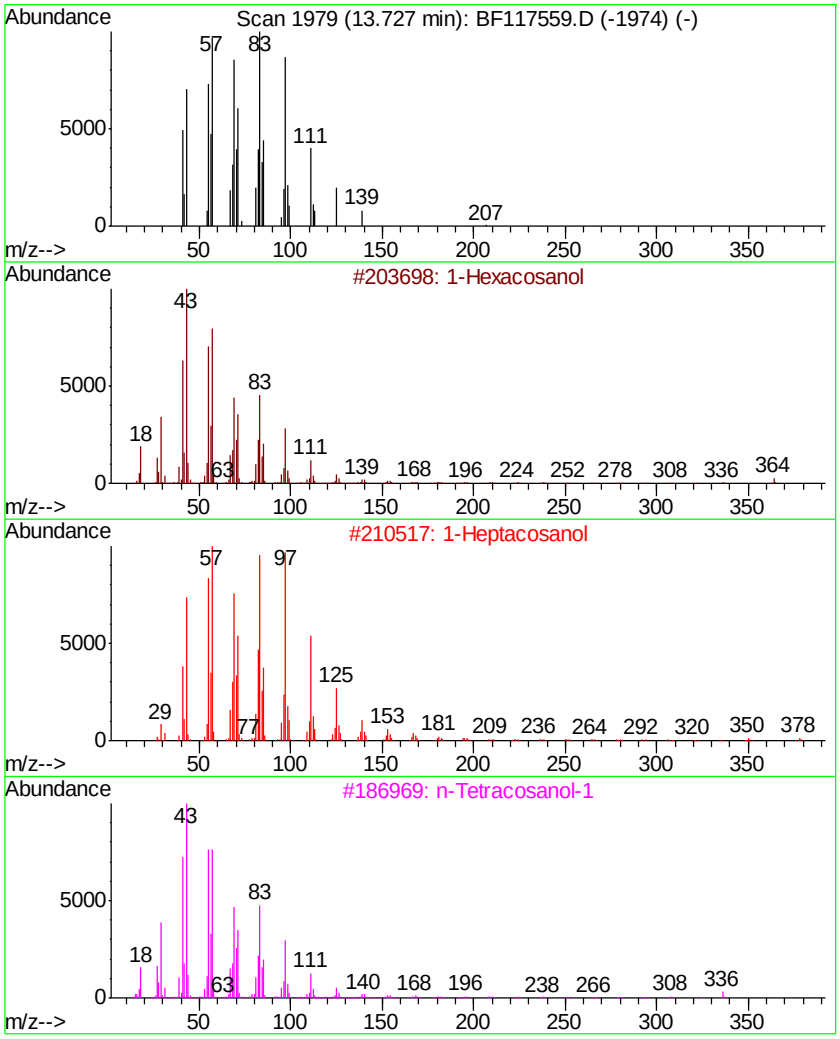
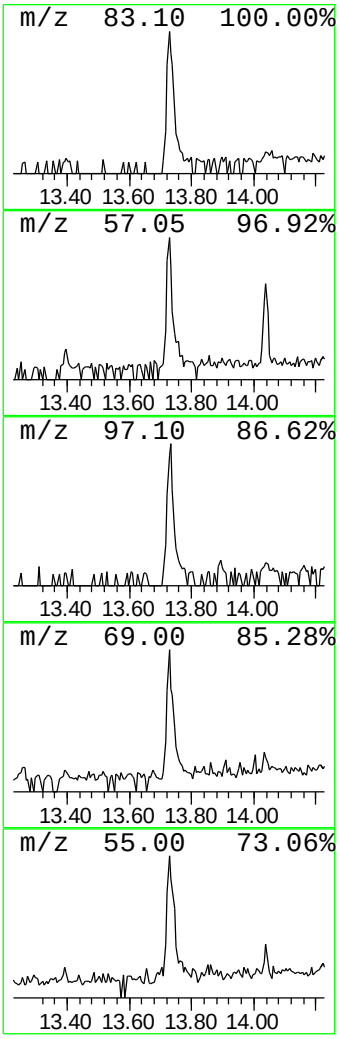
Peak Number 4 1-Hexacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.15 ng	70833	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117559.D
Acq On : 28 Oct 2019 14:16
Operator : JU
Sample : K5501-07
Misc :
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Instrument : BNA_F
ClientSampleId : 186-14-(0-2.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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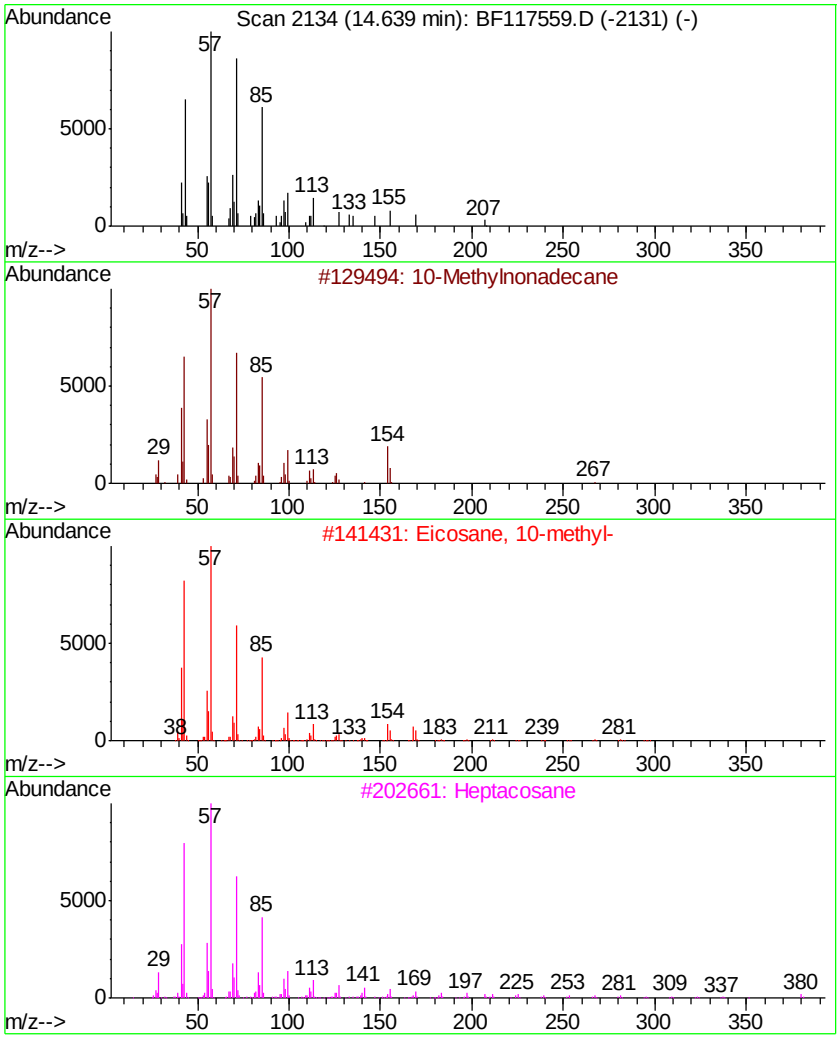
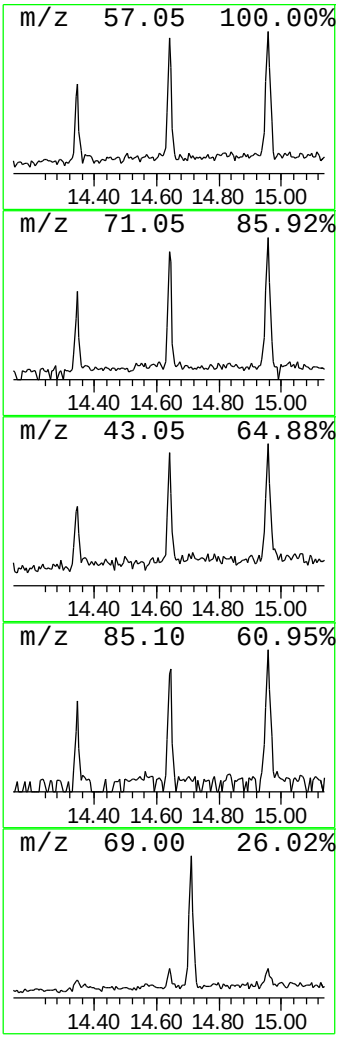
Peak Number 5 10-Methylnonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.85 ng	33641	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	90
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Octacosane	394	C28H58	000630-02-4	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117559.D
Acq On : 28 Oct 2019 14:16
Operator : JU
Sample : K5501-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 186-14-(0-2.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

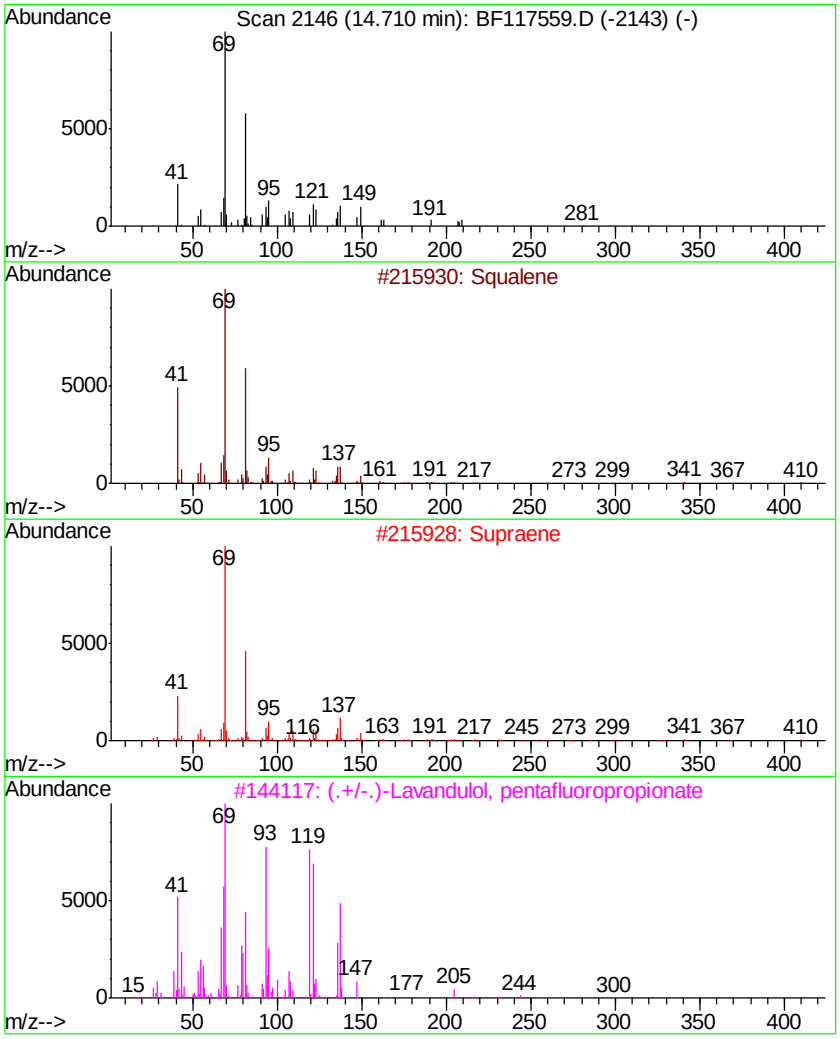
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

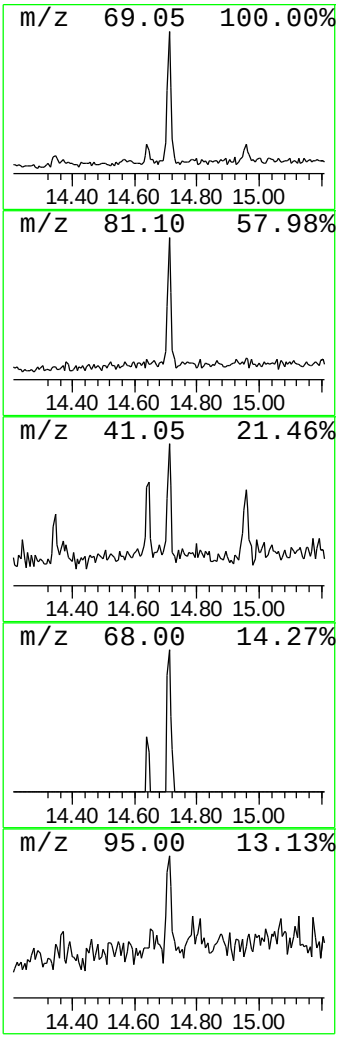
****

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.81 ng	33150	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	86
2	Supraene	410	C30H50	007683-64-9	86
3	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
5	trans-Farnesol	222	C15H26O	000106-28-5	59





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Acq On : 28 Oct 2019 14:16
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 186-14-(0-2.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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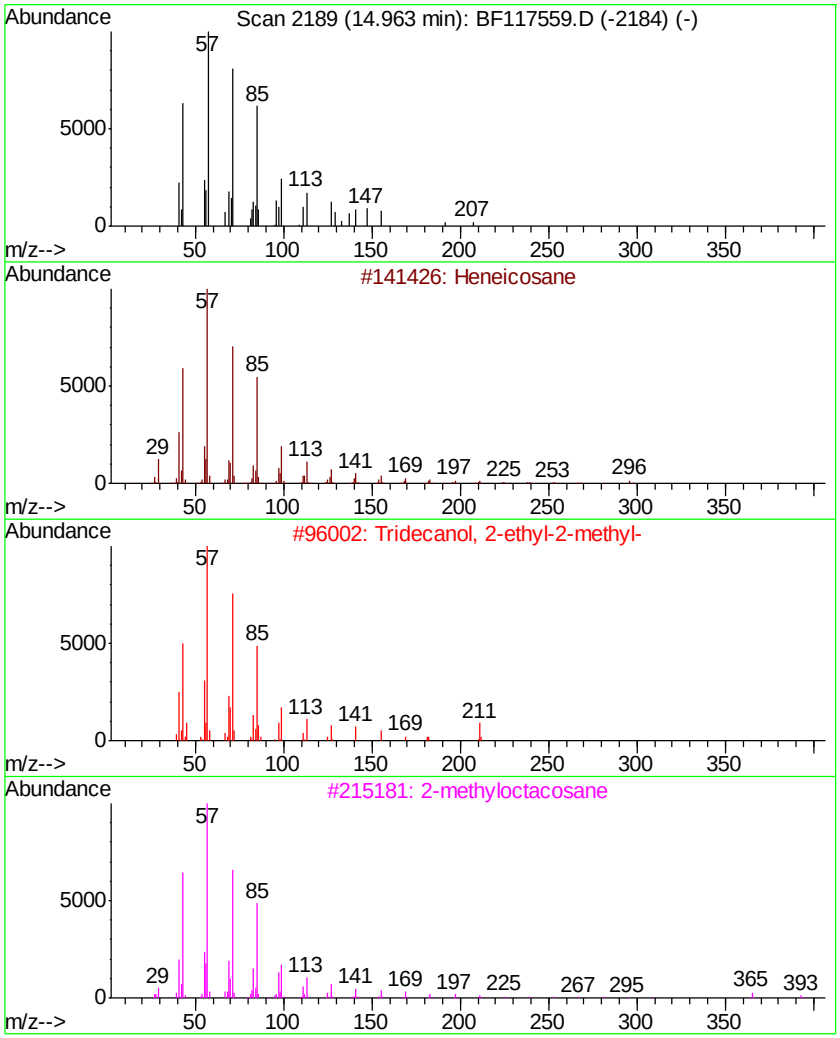
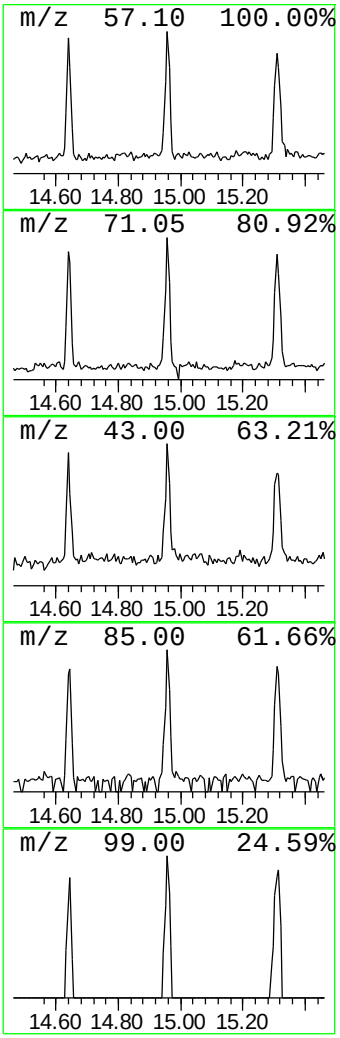
Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.61 ng	42680	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Heptadecane	240	C17H36	000629-78-7	90





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Instrument : BNA_F
ClientSampleId : 186-14-(0-2.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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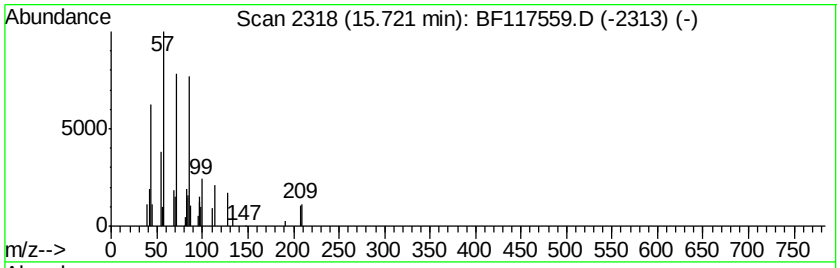
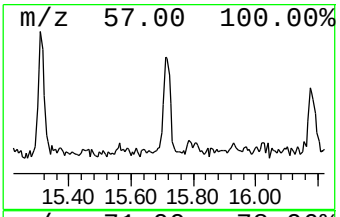
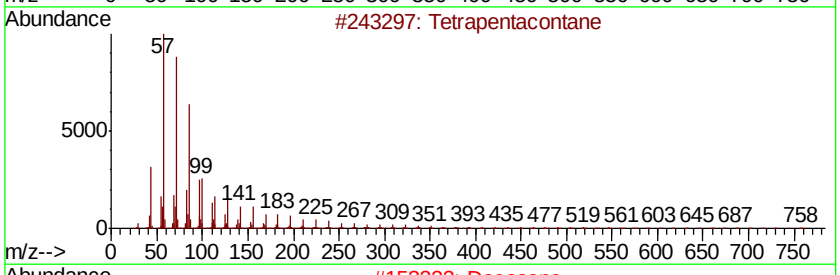
Peak Number 8 Tetrapentacontane Concentration Rank 7

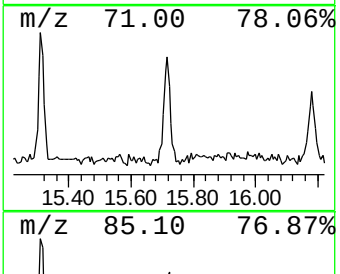
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.51 ng	29657	Perylene-d12	15.33

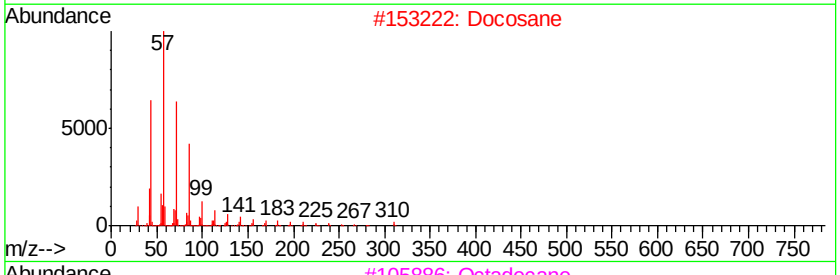
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrapentacontane	759	C54H110	005856-66-6	59
2	Docosane	310	C22H46	000629-97-0	53
3	Octadecane	254	C18H38	000593-45-3	53
4	Heptadecane	240	C17H36	000629-78-7	53
5	Hexatriacontane	507	C36H74	000630-06-8	53

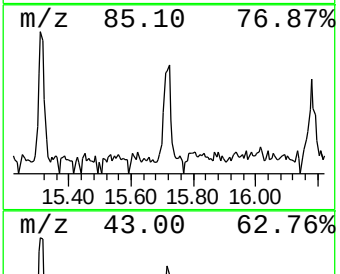


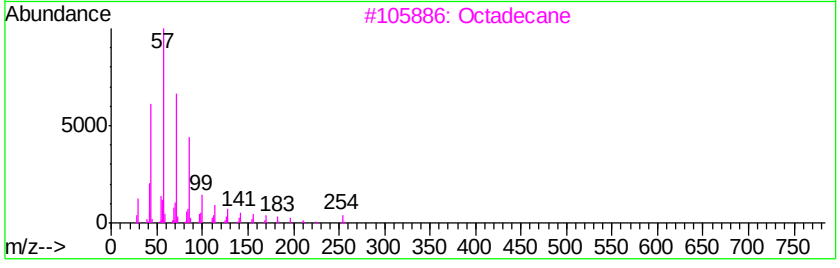


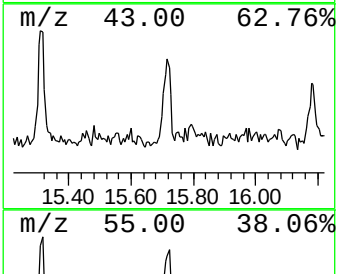


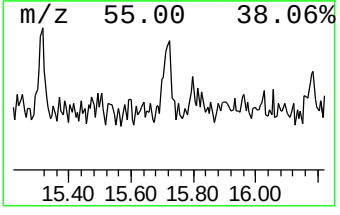












Tentatively Identified Compound (LSC) summary

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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
unknown6.50	6.50	89.1	ng	988020	1	6.73	221763	20.0
Undecanoic acid	11.77	2.2	ng	35549	4	11.25	323424	20.0
1-Hexacosanol	13.73	6.2	ng	70833	5	13.89	230258	20.0
10-Methylnonadecane	14.64	2.9	ng	33641	6	15.33	236265	20.0
Squalene	14.71	2.8	ng	33150	6	15.33	236265	20.0
Heneicosane	14.96	3.6	ng	42680	6	15.33	236265	20.0
Tetrapentacontane	15.72	2.5	ng	29657	6	15.33	236265	20.0