LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

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:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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	5.451	637	640	656	rBV	69700	237165	12.44%	1.755%
2	7.086	915	918	931	rBV	86077	266476	13.98%	1.972%
3	7.181	931	934	947	rVB	160999	388076	20.36%	2.872%
4	7.498	984	988	1002	rBV	536521	791244	41.51%	5.856%
5	7.745	1026	1030	1042	rBV	131735	228076	11.96%	1.688%
6	8.428	1143	1146	1166	rBV	54150	171967	9.02%	1.273%
7	9.527	1329	1333	1347	rBV	725152	1016577	53.33%	7.524%
8	11.304	1631	1635	1646	rBV	273000	348988	18.31%	2.583%
9	11.527	1668	1673	1678	rBV3	17610	27683	1.45%	0.205%
10	11.998	1750	1753	1759	rBV	55319	80813	4.24%	0.598%
11	12.351	1808	1813	1818	rBV2	754457	978150	51.31%	7.240%
12	12.386	1818	1819	1826	rVB	57400	52907	2.78%	0.392%
13	12.910	1904	1908	1914	rVB2	15369	22192	1.16%	0.164%
14	13.198	1953	1957	1962	rVB	71100	80888	4.24%	0.599%
15	13.562	2011	2019	2022	rBV2	31460	61338	3.22%	0.454%
16	13.657	2029	2035	2040	rBV	86530	143684	7.54%	1.063%
17	13.974	2084	2089	2098	rVB	96490	162250	8.51%	1.201%
18	14.704	2208	2213	2216	rBV	106302	128187	6.72%	0.949%
19	14.745	2216	2220	2233	rVB2	693221	972010	50.99%	7.194%
20	15.374	2323	2327	2331	rBV	80642	95835	5.03%	0.709%
21	15.527	2348	2353	2358	rVB	581897	709410	37.22%	5.251%
22	15.980	2425	2430	2436	rVB	76015	91926	4.82%	0.680%
23	16.498	2511	2518	2521	rBV	1140491	1398554	73.37%	10.351%
24	16.533	2521	2524	2527	rVV	1642482	1906212	100.00%	14.109%
25	16.562	2527	2529	2535	rVB2	182042	184425	9.67%	1.365%
26	16.662	2541	2546	2550	rVB	400380	440712	23.12%	3.262%
27	16.733	2550	2558	2562	rBV7	23379	54836	2.88%	0.406%
28	16.974	2594	2599	2604	rVB2	40407	53665	2.82%	0.397%
29	17.027	2604	2608	2612	rBV	47839	59011	3.10%	0.437%
30	17.098	2616	2620	2625	rVB2	217022	239773	12.58%	1.775%
31	17.292	2651	2653	2658	rBV5	17079	25202	1.32%	0.187%
32	17.386	2666	2669	2672	rBV3	32156	41277	2.17%	0.306%
33	17.503	2684	2689	2694	rBV3	44983	76901	4.03%	0.569%
34	17.627	2706	2710	2712	rBV	47548	53718	2.82%	0.398%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

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:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.662	2713	2716	2720	rVB4	20676	25038	1.31%	0.185%
36	17.756	2729	2732	2736	rBV5	22540	32136	1.69%	0.238%
37	17.945	2761	2764	2768	rVB2	27029	31511	1.65%	0.233%
38	18.168	2797	2802	2805	rVB7	21373	34727	1.82%	0.257%
39	18.368	2833	2836	2841	rVB	20761	23220	1.22%	0.172%
40	18.445	2845	2849	2853	rBV	525825	619530	32.50%	4.585%
41	18.480	2853	2855	2859	rVB2	43835	50476	2.65%	0.374%
42	19.521	3029	3032	3035	rBV3	24794	29141	1.53%	0.216%
43	19.633	3047	3051	3054	rBV	27485	41128	2.16%	0.304%
44	20.109	3128	3132	3141	rBV	424735	563891	29.58%	4.174%
45	20.562	3207	3209	3214	rBV	53231	57117	3.00%	0.423%
46	20.656	3223	3225	3230	rVB5	64190	78797	4.13%	0.583%
47	20.703	3231	3233	3235	rBV3	26712	34262	1.80%	0.254%
48	20.827	3252	3254	3256	rBV3	22085	21744	1.14%	0.161%
49	20.903	3264	3267	3269	rBV4	28124	38393	2.01%	0.284%
50	21.115	3301	3303	3304	rBV2	26217	19587	1.03%	0.145%
51	21.350	3341	3343	3346	rBV3	31758	40247	2.11%	0.298%
52	21.503	3366	3369	3373	rBV4	40557	73622	3.86%	0.545%
53	21.733	3407	3408	3410	rBV2	31770	31325	1.64%	0.232%
54	22.703	3571	3573	3576	rBV3	26820	29212	1.53%	0.216%
55	22.756	3579	3582	3583	rBV3	26941	25348	1.33%	0.188%
56	23.385	3687	3689	3693	rVB5	18188	20079	1.05%	0.149%

Sum of corrected areas: 13510659

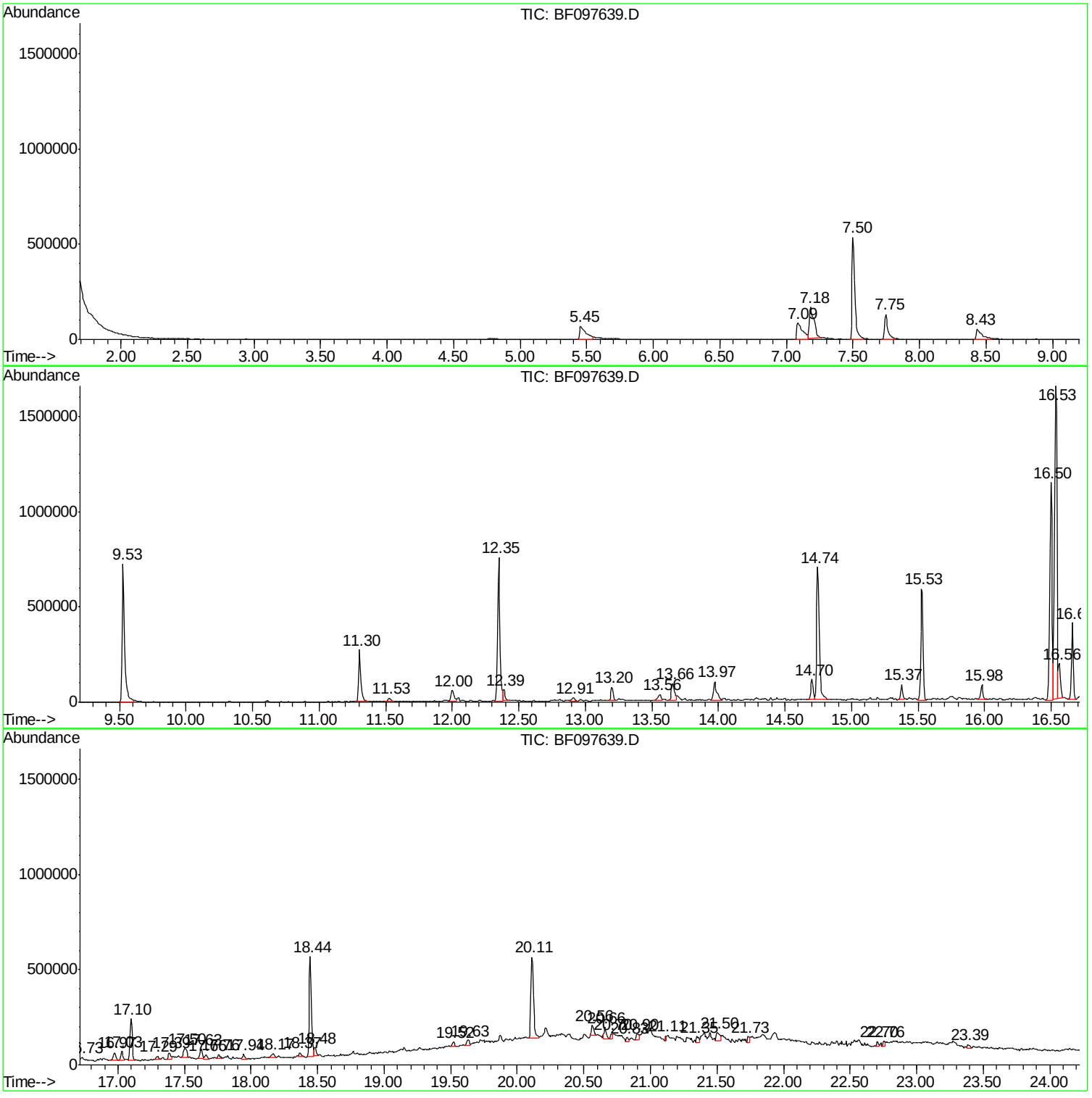
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

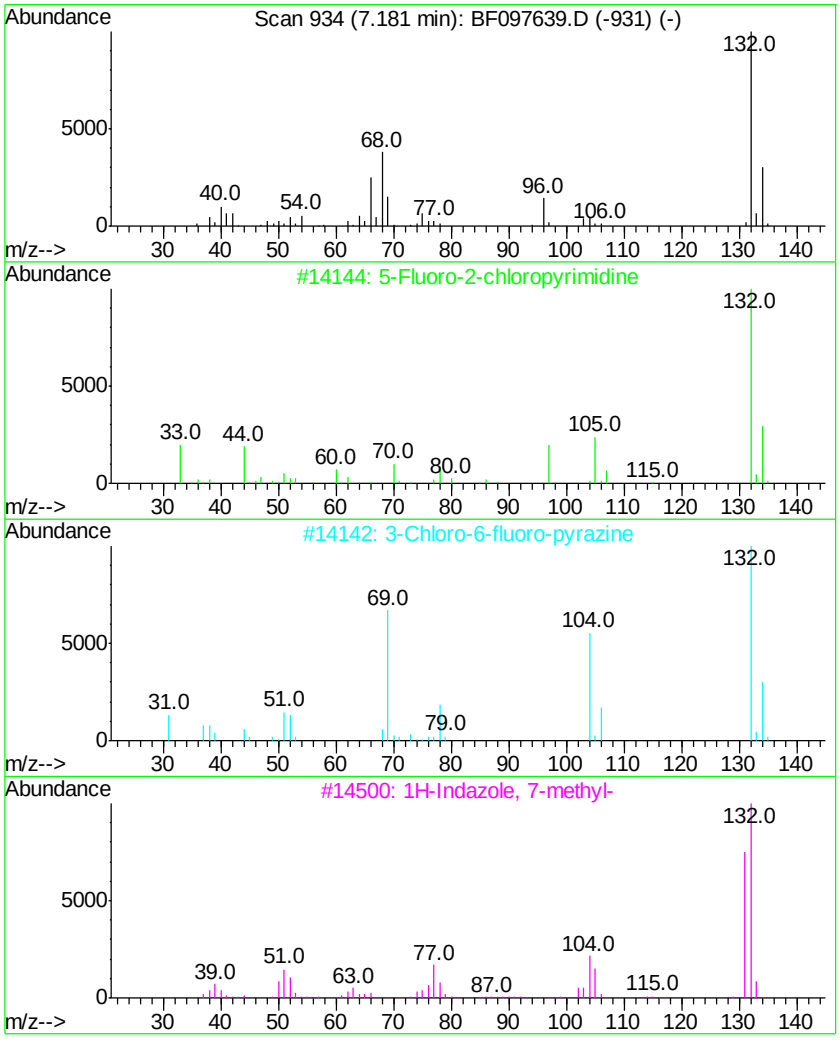
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

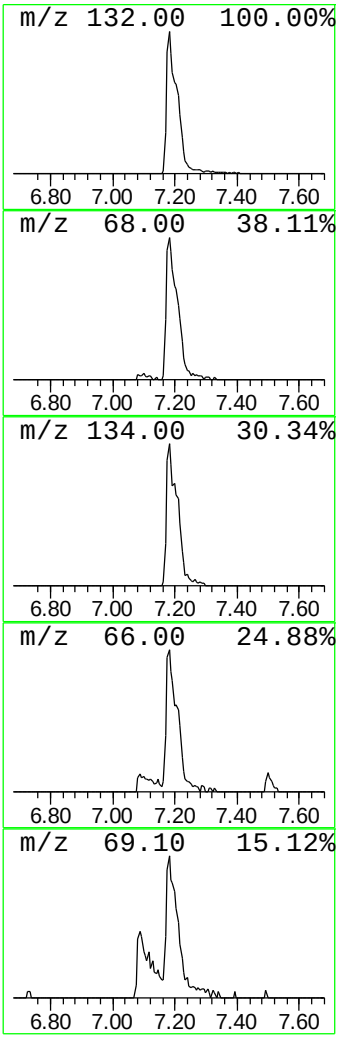
****

Peak Number 1 unknown7.18 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.18	9.81 ng	388076	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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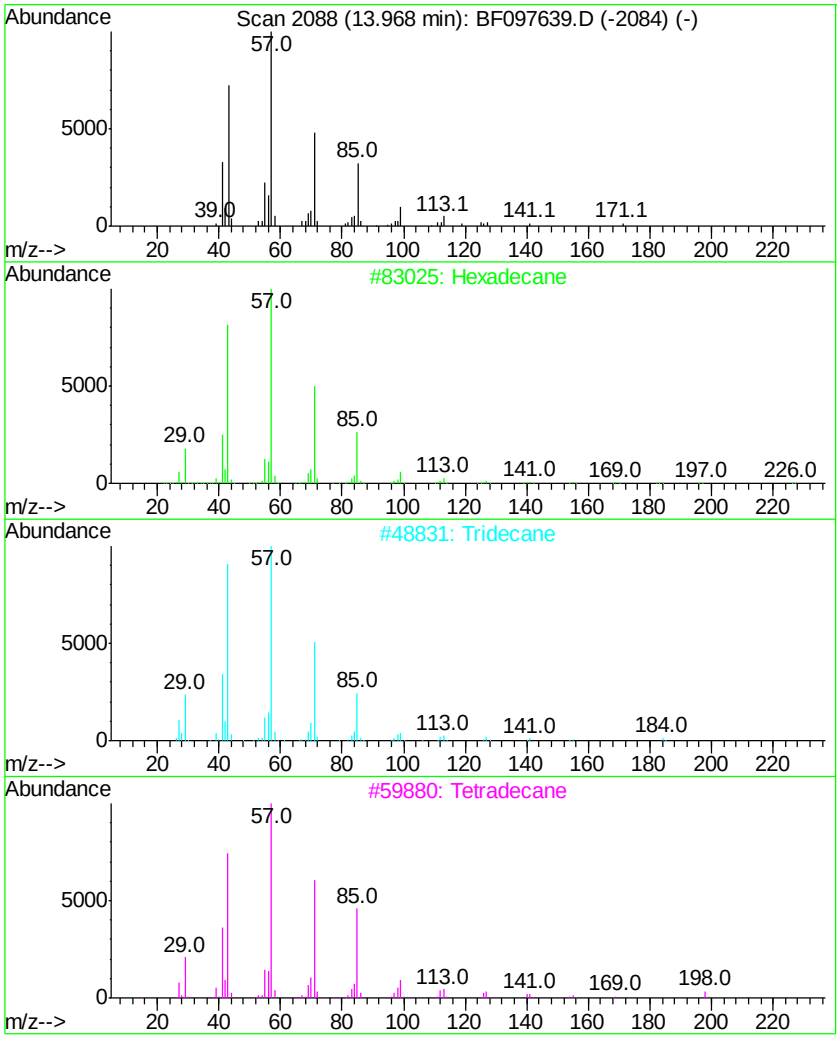
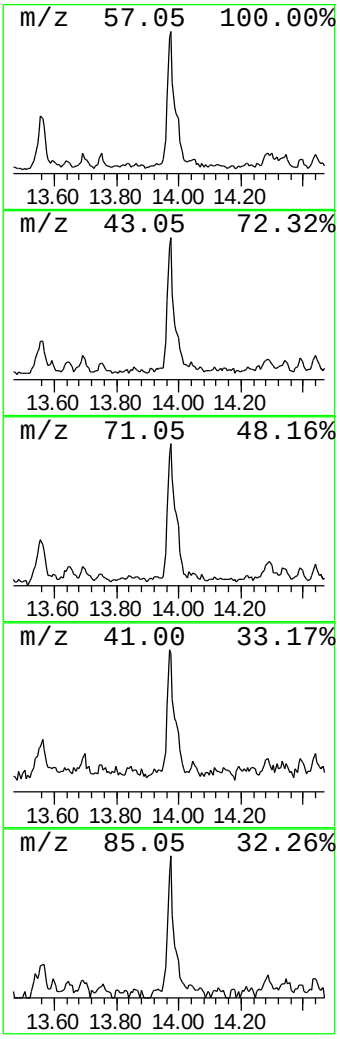
Peak Number 3 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.34 ng	162250	Phenanthrene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tridecane	184	C13H28	000629-50-5	83
3	Tetradecane	198	C14H30	000629-59-4	80
4	Pentadecane	212	C15H32	000629-62-9	80
5	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

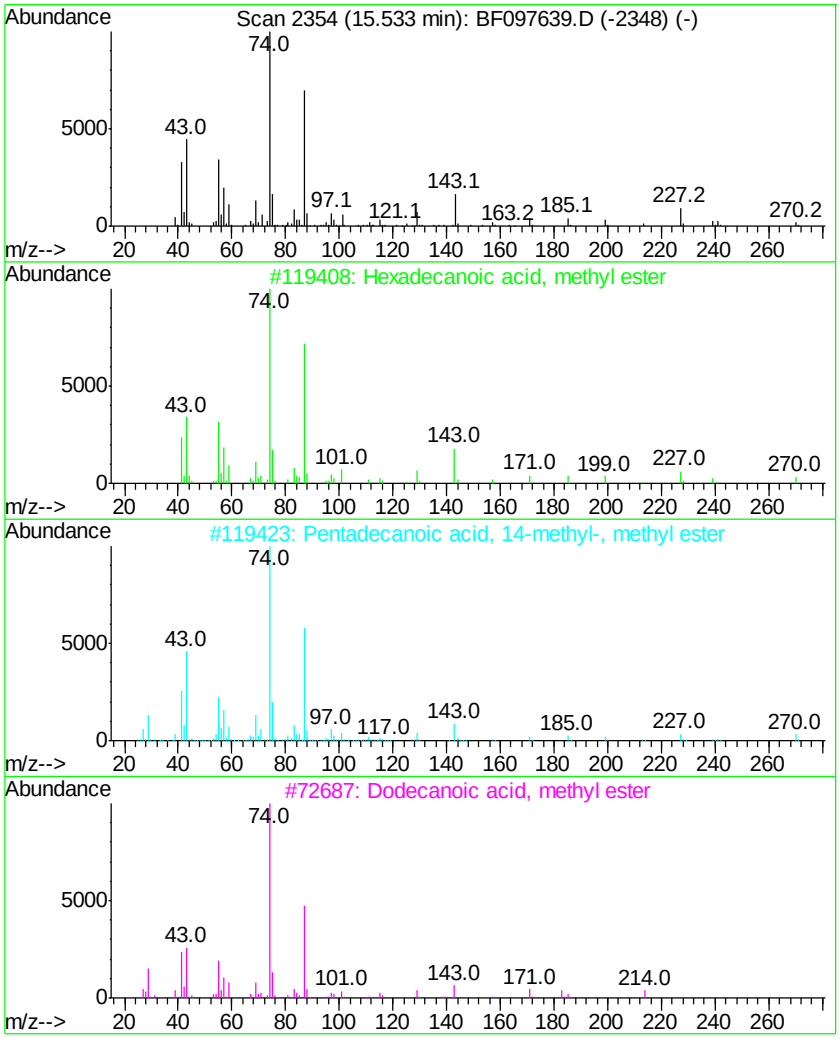
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

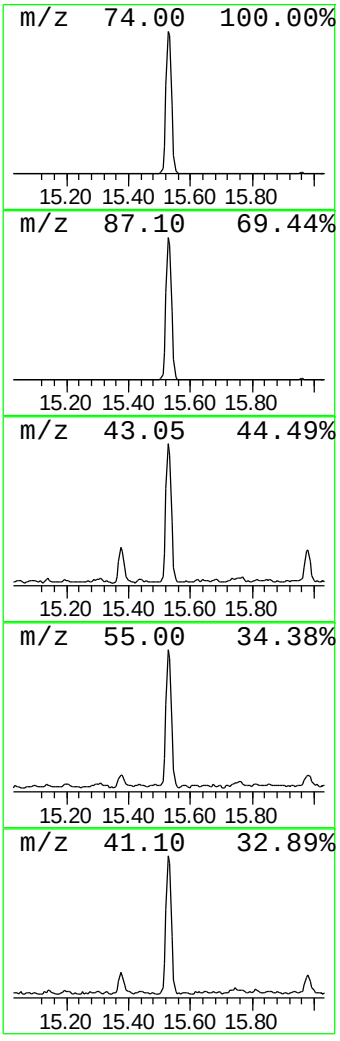
****

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	14.60 ng	709410	Phenanthrene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	90
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

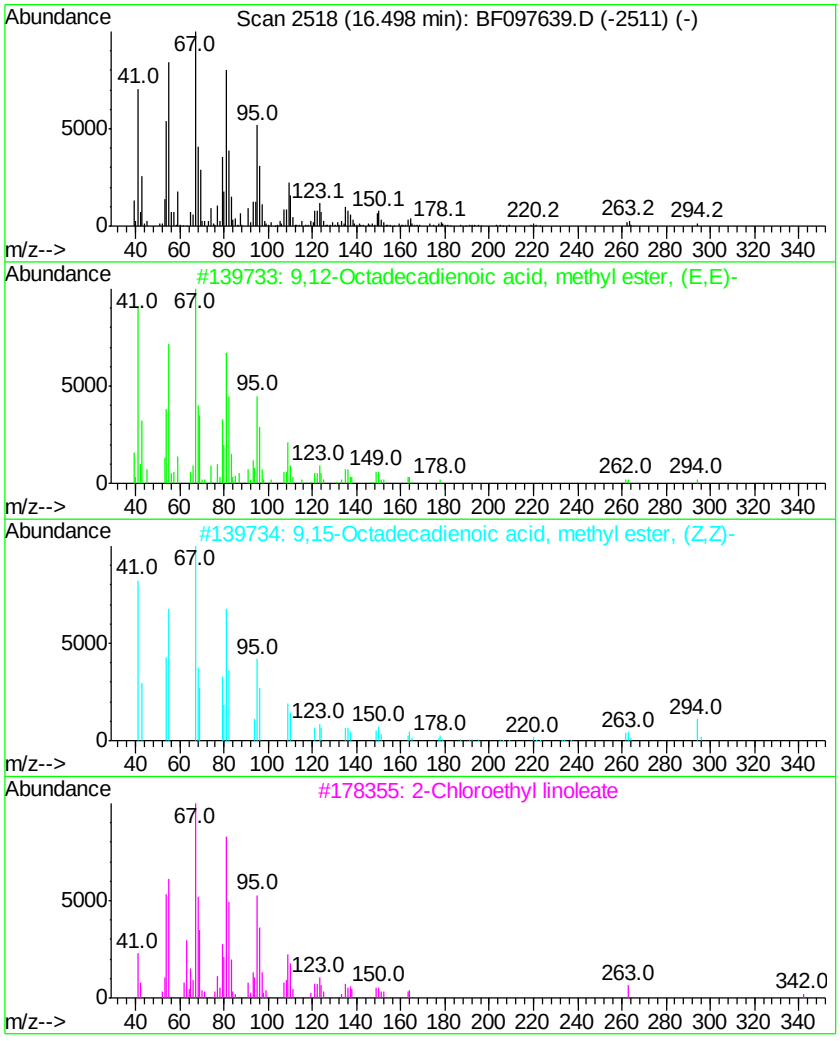
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

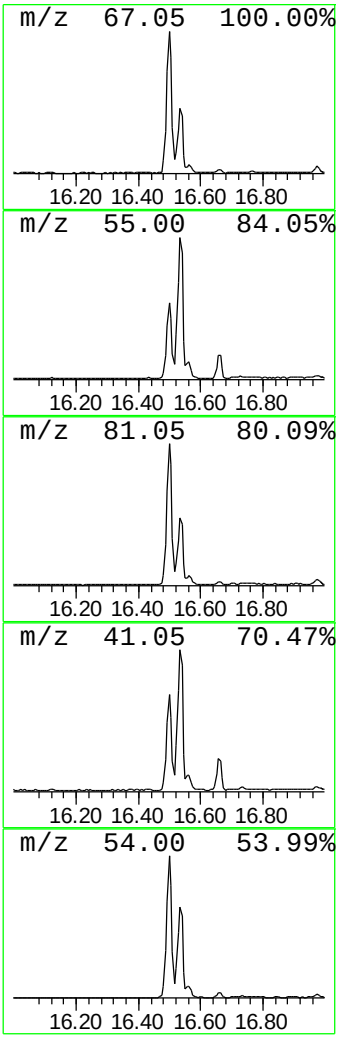
****

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	28.78 ng	1398550	Phenanthrene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	95
3	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	94
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	93
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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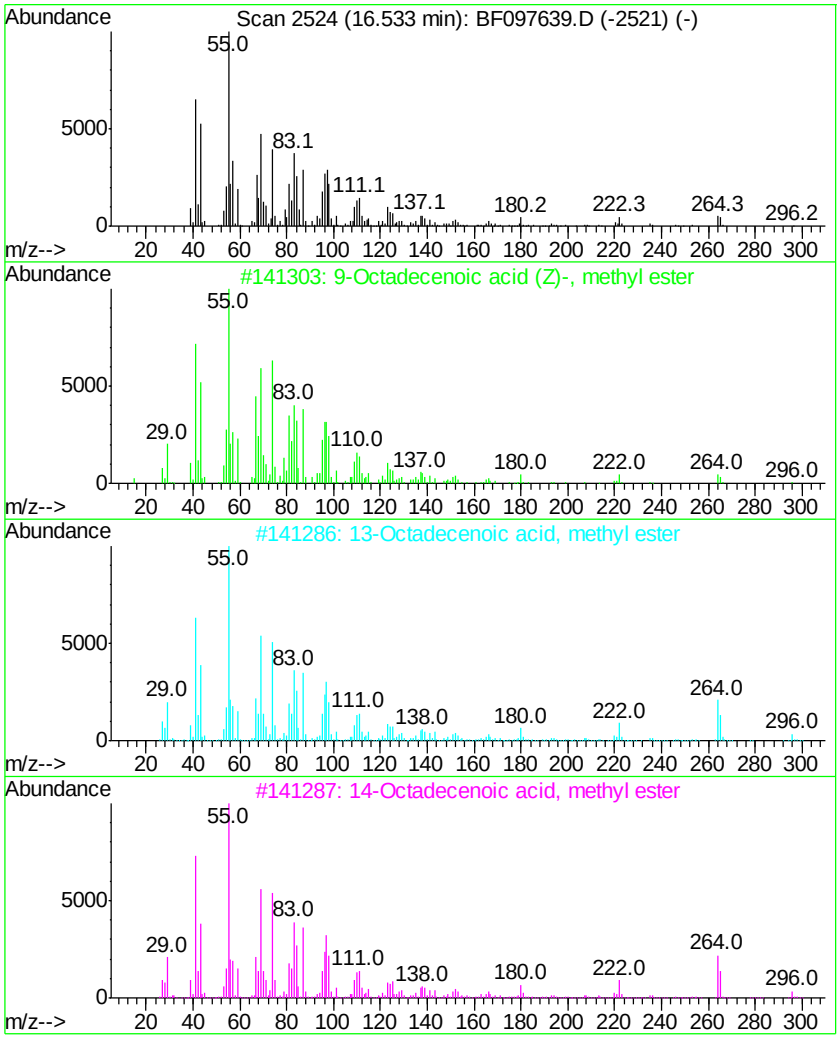
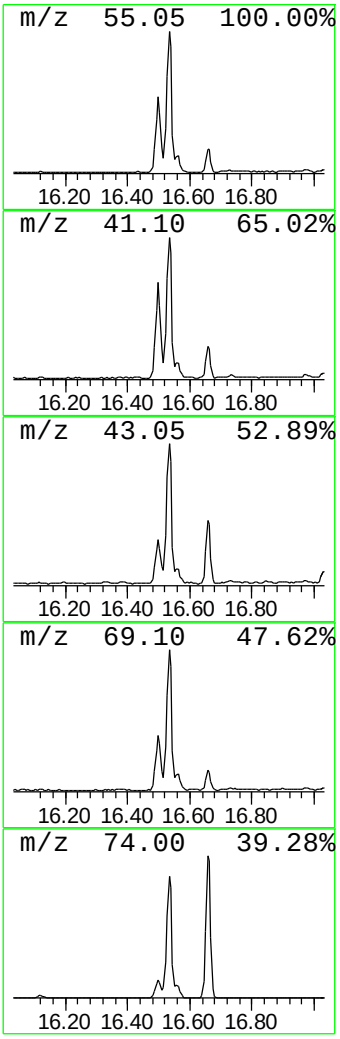
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	39.22 ng	1906210	Phenanthrene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	98
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	97
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	94
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	93





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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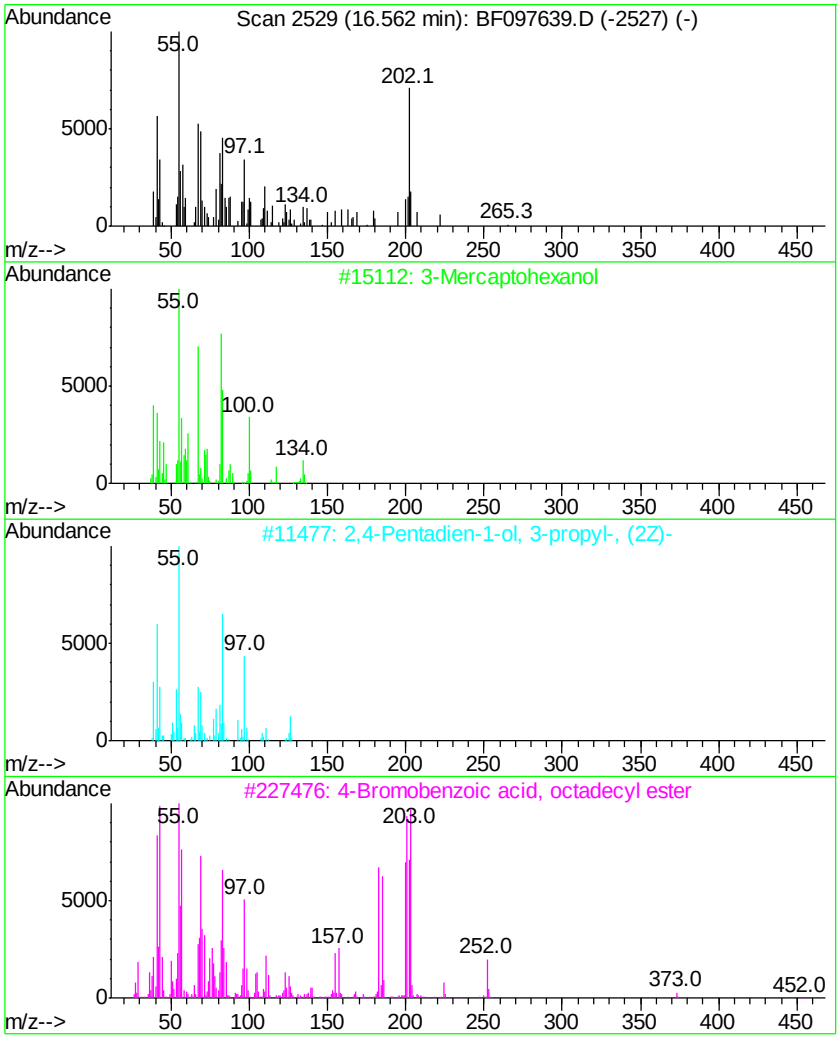
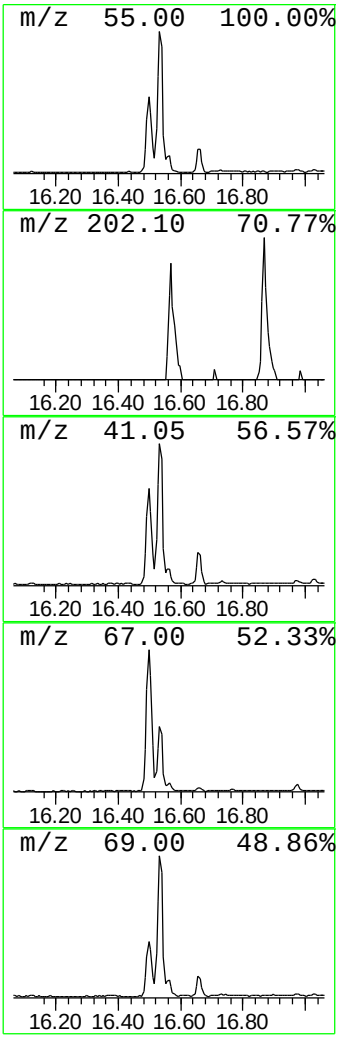
Peak Number 7 unknown16.56 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	3.79 ng	184425	Phenanthrene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Mercaptohexanol	134	C6H14OS	051755-83-0	27
2	2,4-Pentadien-1-ol, 3-propyl-, (...	126	C8H14O	1000142-17-9	25
3	4-Bromobenzoic acid, octadecyl e...	452	C25H41BrO2	070153-15-0	22
4	4-Octyne	110	C8H14	001942-45-6	18
5	Fluoranthene	202	C16H10	000206-44-0	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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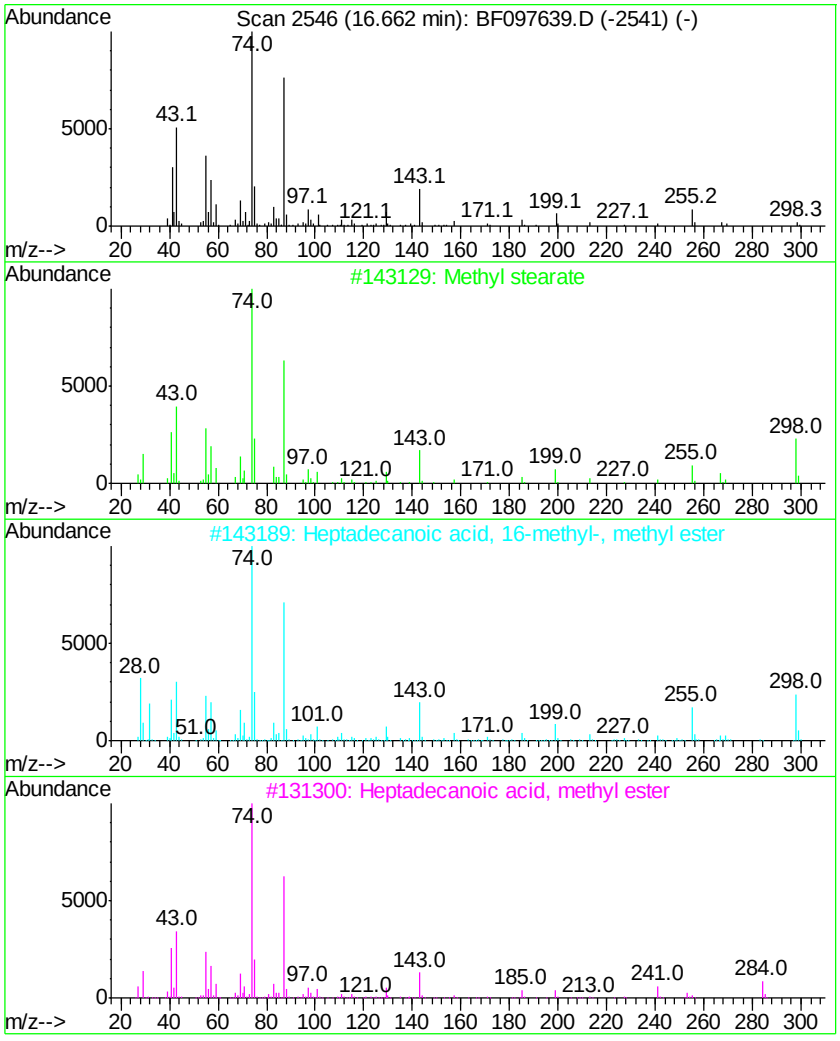
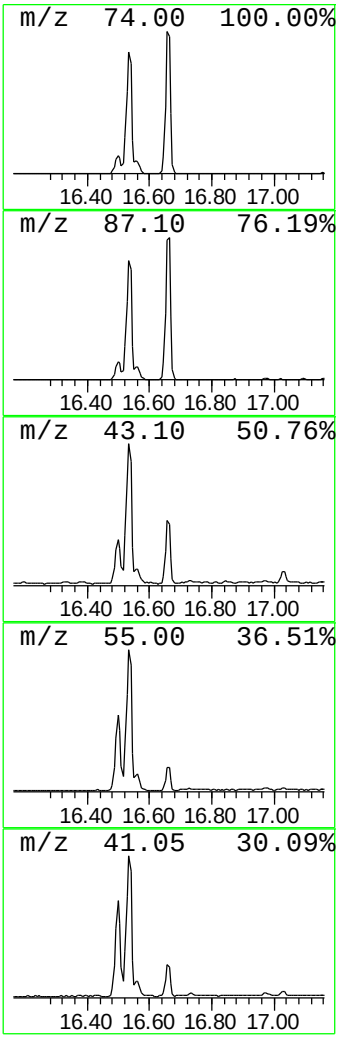
Peak Number 8 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	14.23 ng	440712	Chrysene-d12	18.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	97
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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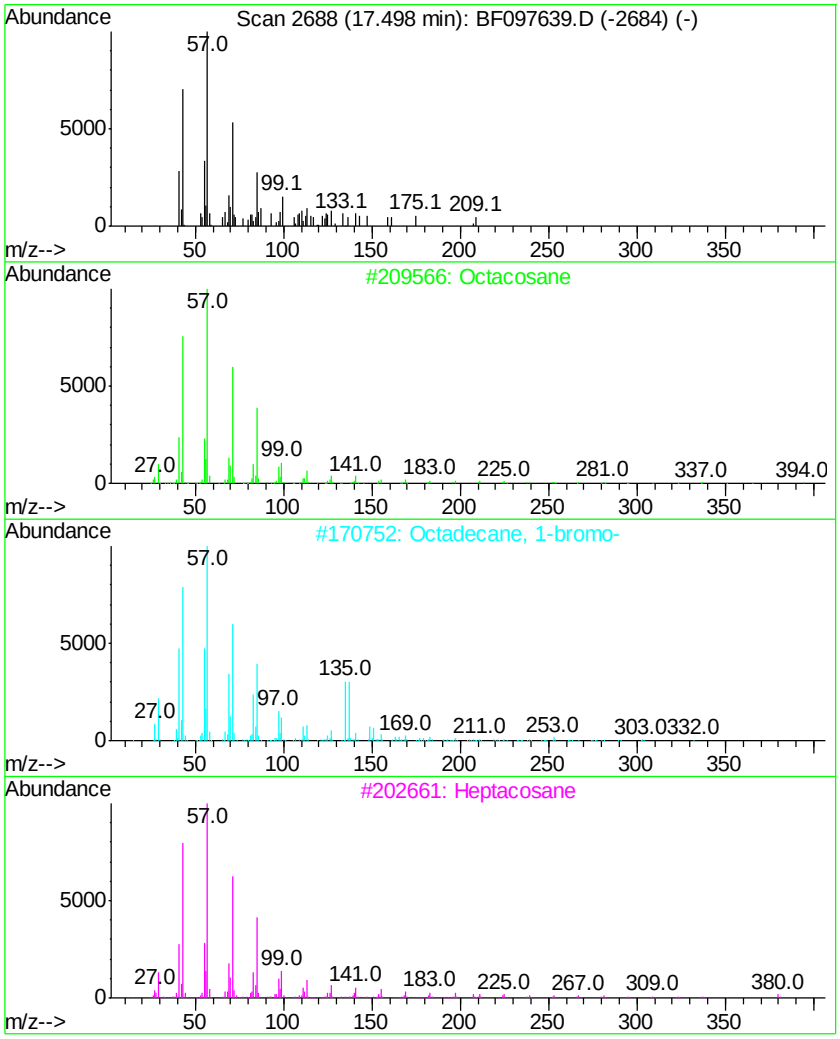
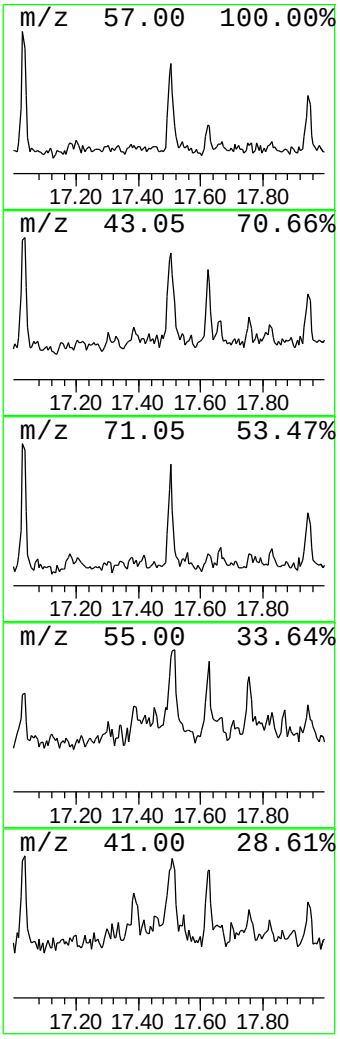
Peak Number 9 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.50	2.48 ng	76901	Chrysene-d12	18.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	72
2	Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	72
3	Heptacosane	380	C27H56	000593-49-7	72
4	Tetracosane	338	C24H50	000646-31-1	72
5	Hexadecane	226	C16H34	000544-76-3	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

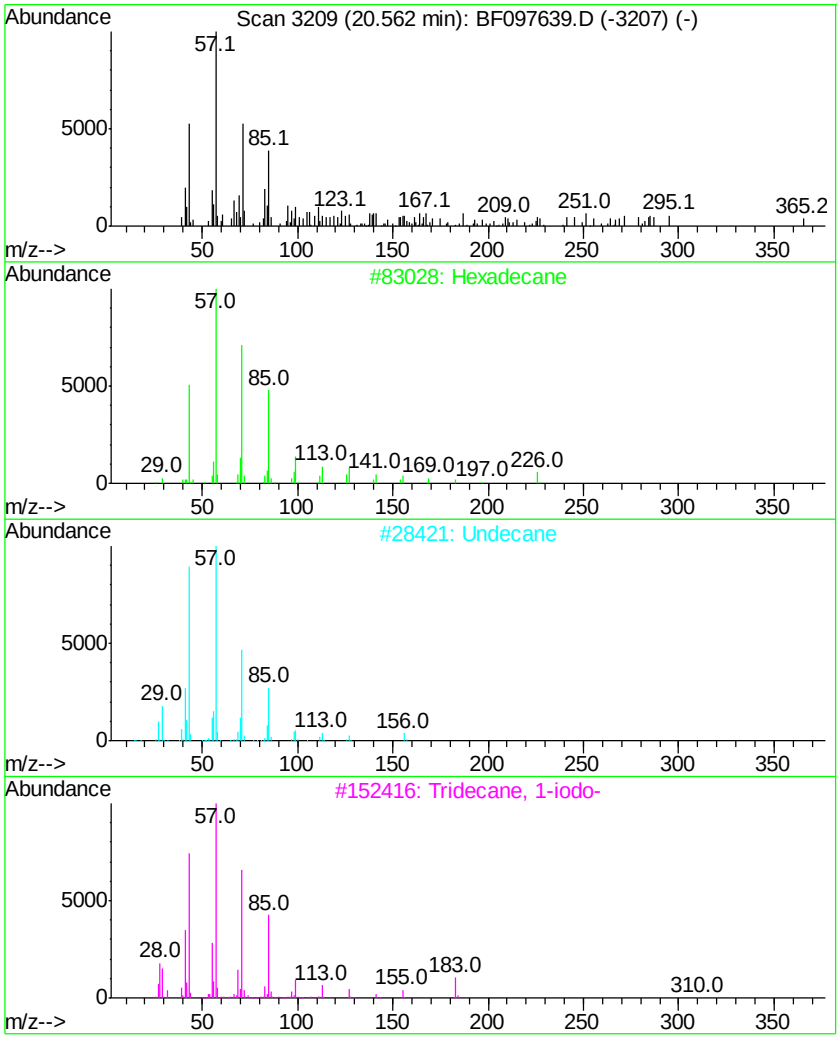
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

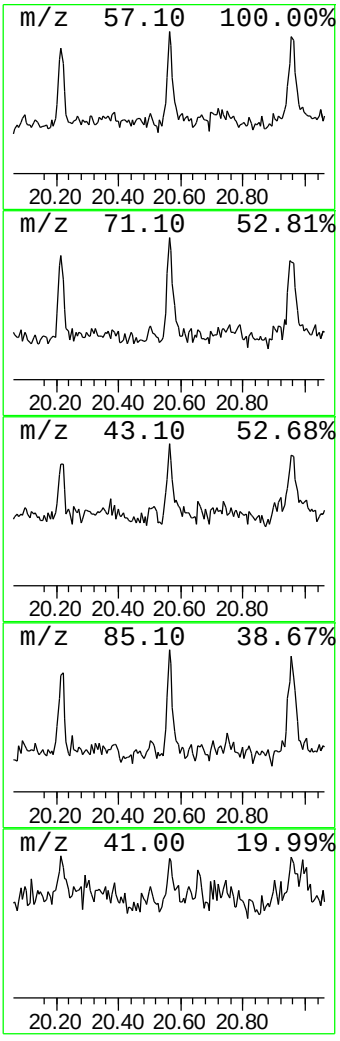
****

Peak Number 10 Undecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.56	2.03 ng	57117	Perylene-d12	20.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	64
2	Undecane	156	C11H24	001120-21-4	58
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	52
4	Tetradecane	198	C14H30	000629-59-4	52
5	Nonadecane	268	C19H40	000629-92-5	52





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
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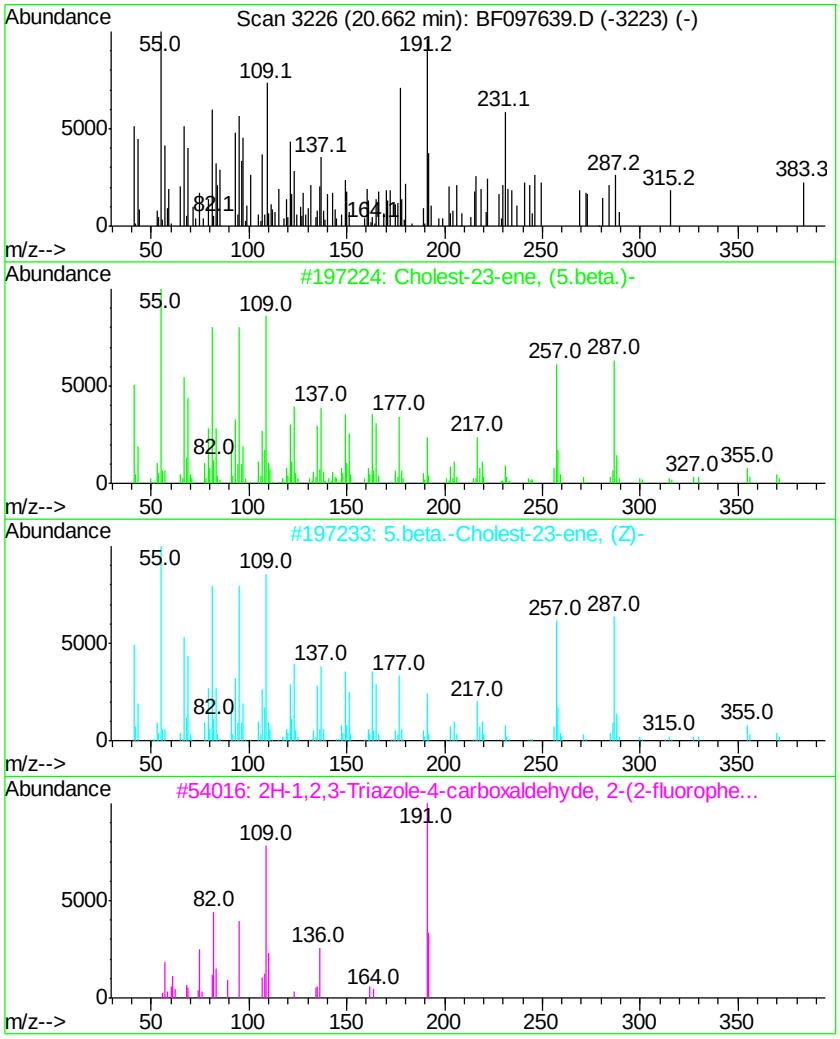
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

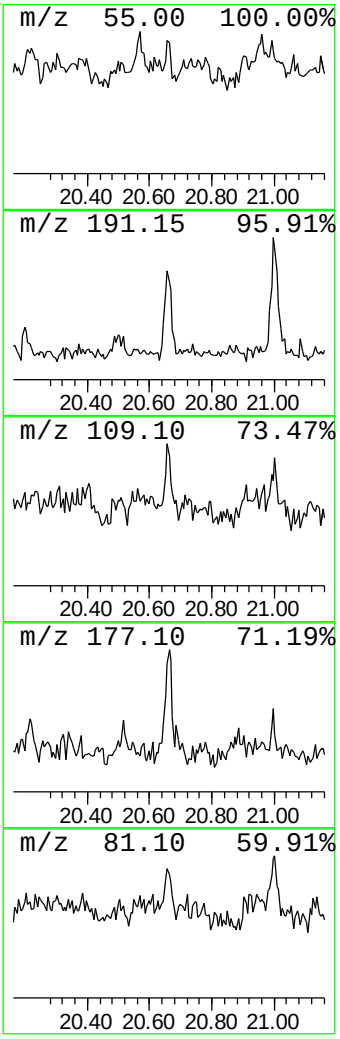
****

Peak Number 11 unknown20.66 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.66	2.79 ng	78797	Perylene-d12	20.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-23-ene, (5.beta.)-	370	C27H46	030658-62-9	43
2	5.beta.-Cholest-23-ene, (Z)-	370	C27H46	014949-12-3	43
3	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	35
4	5-(7a-Isopropenyl-4,5-dimethyl-o...	290	C20H34O	1000193-54-0	30
5	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

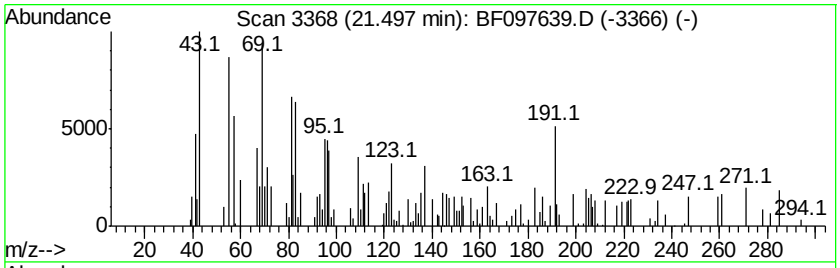
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

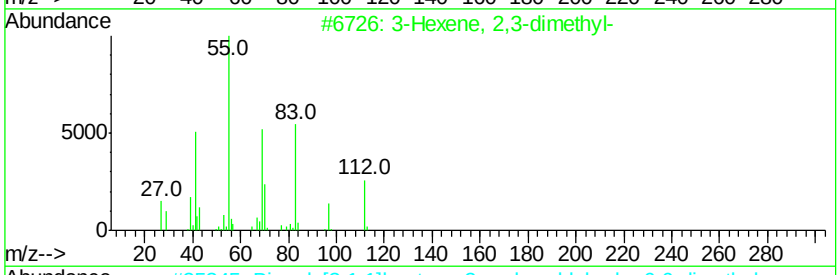
****

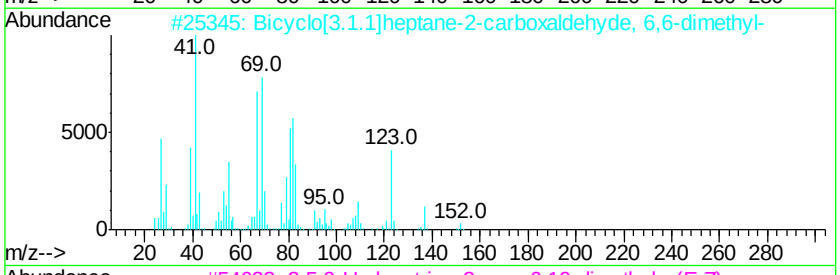
Peak Number 12 unknown21.50 Concentration Rank 10

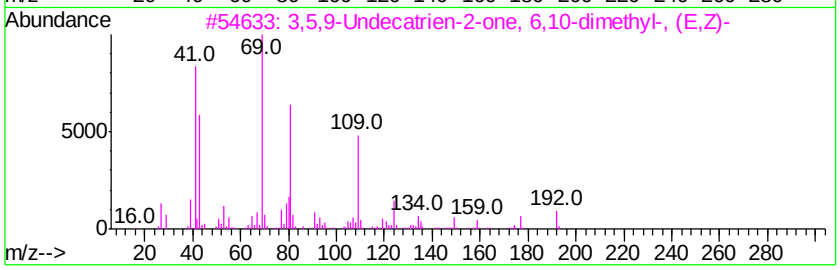
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	2.61 ng	73622	Perylene-d12	20.11

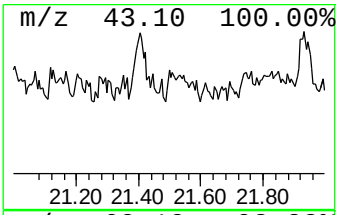
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexene, 2,3-dimethyl-	112	C8H16	007145-23-5	25
2	Bicyclo[3.1.1]heptane-2-carboxal...	152	C10H16O	004764-14-1	25
3	3,5,9-Undecatrien-2-one, 6,10-di...	192	C13H20O	013927-47-4	20
4	Dicyclohexylcarbodiimide	206	C13H22N2	000538-75-0	15
5	3-Ethyl-4-methyl-2-pentene	112	C8H16	019780-68-8	11

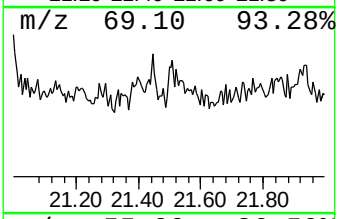


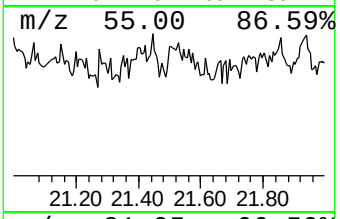


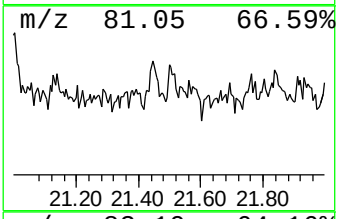


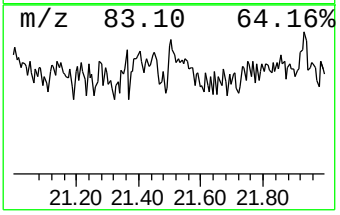












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097639.D
Acq On : 12 Aug 2017 17:36
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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
unknown7.18	7.18	9.8	ng	388076	1	7.50	791244	20.0
Hexadecane	13.97	3.3	ng	162250	4	14.74	972010	20.0
Hexadecanoic acid...	15.53	14.6	ng	709410	4	14.74	972010	20.0
9,12-Octadecadien...	16.50	28.8	ng	1398550	4	14.74	972010	20.0
9-Octadecenoic ac...	16.53	39.2	ng	1906210	4	14.74	972010	20.0
unknown16.56	16.56	3.8	ng	184425	4	14.74	972010	20.0
Methyl stearate	16.66	14.2	ng	440712	5	18.44	619530	20.0
Octacosane	17.50	2.5	ng	76901	5	18.44	619530	20.0
Undecane	20.56	2.0	ng	57117	6	20.11	563891	20.0
unknown20.66	20.66	2.8	ng	78797	6	20.11	563891	20.0
unknown21.50	21.50	2.6	ng	73622	6	20.11	563891	20.0