LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097688.D
Acq On : 15 Aug 2017 13:53
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

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-BF081517.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	4.981	487	492	500	rVB	194080	273769	9.82%	0.874%
2	5.387	556	561	564	rBV	2586942	2603839	93.41%	8.315%
3	6.410	729	735	739	rVB	2564014	2765894	99.22%	8.833%
4	6.551	754	759	762	rBV	2559256	2607378	93.53%	8.326%
5	6.781	794	798	802	rBV	1100462	856257	30.72%	2.734%
6	6.939	820	825	828	rBV	2036280	1798366	64.51%	5.743%
7	7.345	889	894	897	rBV	1648338	1623777	58.25%	5.185%
8	7.428	903	908	911	rBV	38109	35806	1.28%	0.114%
9	8.063	1012	1016	1019	rBV	1376049	1130456	40.55%	3.610%
10	8.775	1133	1137	1140	rBV	40188	29485	1.06%	0.094%
11	9.139	1195	1199	1203	rBV	2814495	2607274	93.53%	8.326%
12	9.533	1263	1266	1270	rBV	610079	496723	17.82%	1.586%
13	9.757	1301	1304	1309	rVB2	36697	32560	1.17%	0.104%
14	9.816	1310	1314	1318	rBV2	1277349	1110987	39.85%	3.548%
15	10.022	1346	1349	1352	rBV	35707	31073	1.11%	0.099%
16	10.257	1386	1389	1392	rVB	72961	51929	1.86%	0.166%
17	10.480	1420	1427	1429	rBV	22840	33622	1.21%	0.107%
18	10.598	1443	1447	1451	rBV	1556655	1467744	52.65%	4.687%
19	10.727	1466	1469	1478	rBV	82355	101465	3.64%	0.324%
20	10.969	1507	1510	1513	rBV3	28455	30541	1.10%	0.098%
21	11.180	1542	1546	1548	rBV2	53079	42826	1.54%	0.137%
22	11.298	1562	1566	1569	rBV	1240461	1035530	37.15%	3.307%
23	11.322	1569	1570	1572	rVV	65590	30012	1.08%	0.096%
24	11.369	1572	1578	1581	rVB3	37985	36339	1.30%	0.116%
25	11.857	1652	1661	1668	rBV	2154392	2787620	100.00%	8.902%
26	12.233	1722	1725	1730	rBV4	25196	31311	1.12%	0.100%
27	12.427	1756	1758	1764	rVB4	22782	29699	1.07%	0.095%
28	12.504	1766	1771	1774	rBV	148652	146785	5.27%	0.469%
29	12.551	1775	1779	1781	rBV4	25633	35124	1.26%	0.112%
30	12.633	1786	1793	1805	rVV	1752550	2059785	73.89%	6.578%
31	12.733	1805	1810	1813	rVB	124567	143104	5.13%	0.457%
32	12.886	1832	1836	1839	rBV	2126982	1872909	67.19%	5.981%
33	13.339	1911	1913	1916	rBV4	25632	30925	1.11%	0.099%
34	13.727	1974	1979	1982	rBV3	40254	64690	2.32%	0.207%

LSC Area Percent Report

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Acq On : 15 Aug 2017 13:53
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.763	1982	1985	1987	rVV	26297	28688	1.03%	0.092%
36	13.792	1987	1990	1995	rVV2	344203	352814	12.66%	1.127%
37	13.927	2008	2013	2016	rBV	856244	898957	32.25%	2.871%
38	13.957	2016	2018	2020	rVB	53586	44057	1.58%	0.141%
39	14.115	2042	2045	2053	rBV6	25954	47732	1.71%	0.152%
40	14.427	2093	2098	2102	rBV	131428	162877	5.84%	0.520%
41	14.727	2146	2149	2155	rVB4	23240	35325	1.27%	0.113%
42	14.792	2157	2160	2164	rVB	39785	49479	1.77%	0.158%
43	14.945	2183	2186	2189	rBV	67956	88506	3.17%	0.283%
44	15.051	2201	2204	2212	rBV4	56952	100567	3.61%	0.321%
45	15.239	2232	2236	2240	rBV	44878	54801	1.97%	0.175%
46	15.298	2242	2246	2251	rBV	40877	53861	1.93%	0.172%
47	15.362	2251	2257	2264	rBV	598268	753532	27.03%	2.406%
48	15.851	2336	2340	2343	rBV	42923	68176	2.45%	0.218%
49	15.886	2343	2346	2355	rVB6	45487	85675	3.07%	0.274%
50	16.209	2399	2401	2408	rVB6	25612	44597	1.60%	0.142%
51	16.745	2489	2492	2502	rVB4	15651	33747	1.21%	0.108%
52	17.345	2586	2594	2603	rVV10	56895	144096	5.17%	0.460%
53	17.439	2606	2610	2618	rVB8	21866	47035	1.69%	0.150%
54	19.327	2923	2931	2941	rBV9	56050	184311	6.61%	0.589%

Sum of corrected areas: 31314437

LSC Report - Integrated Chromatogram

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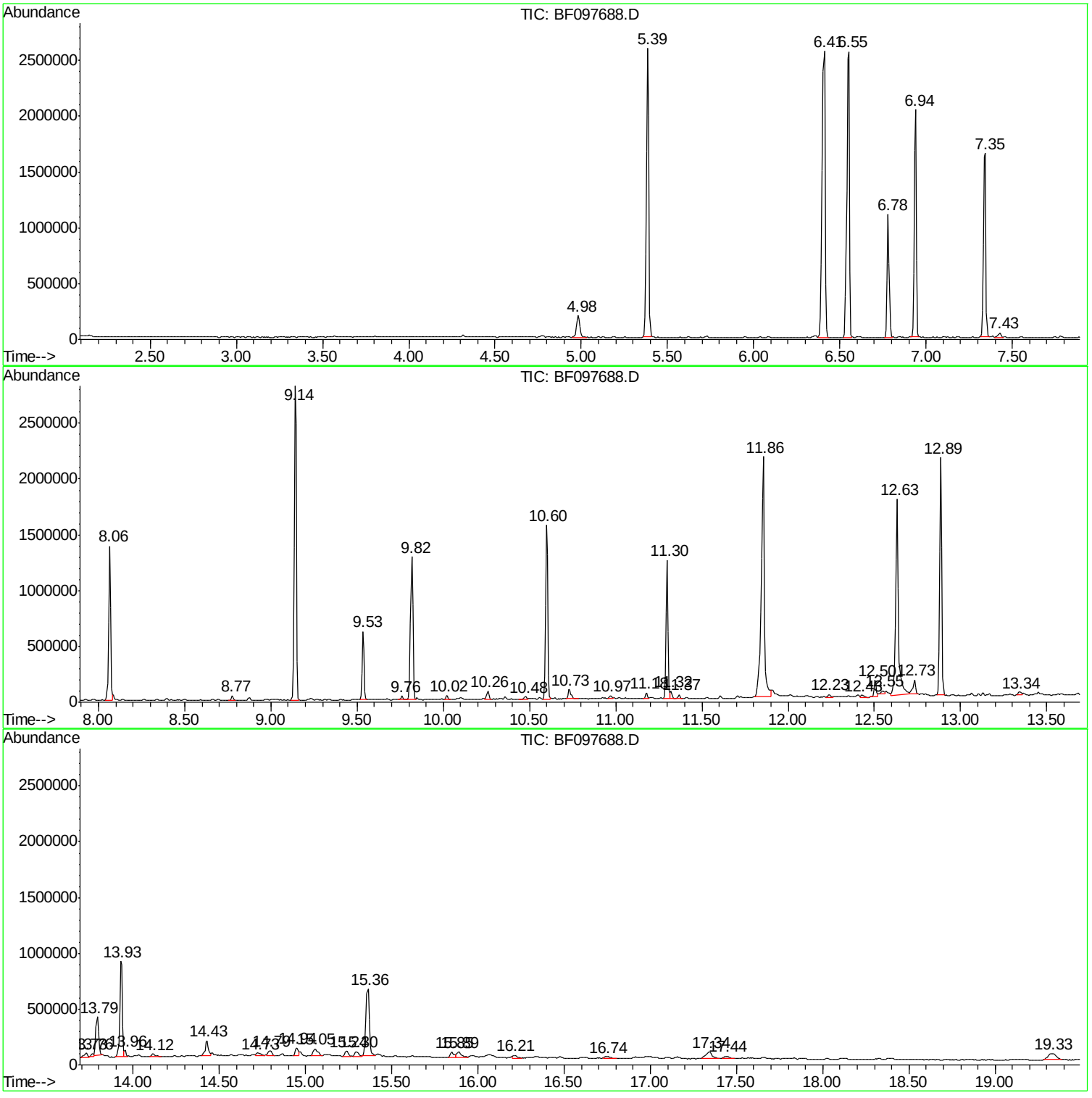
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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\BF081517\
Data File : BF097688.D
Acq On : 15 Aug 2017 13:53
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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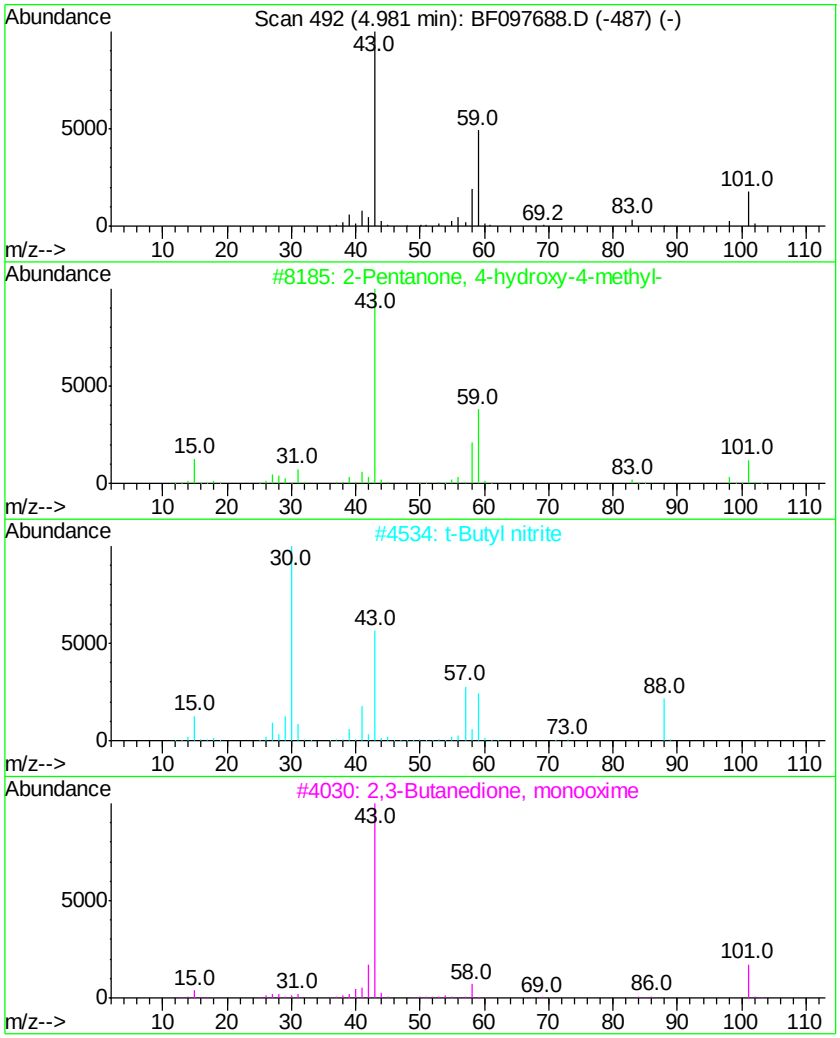
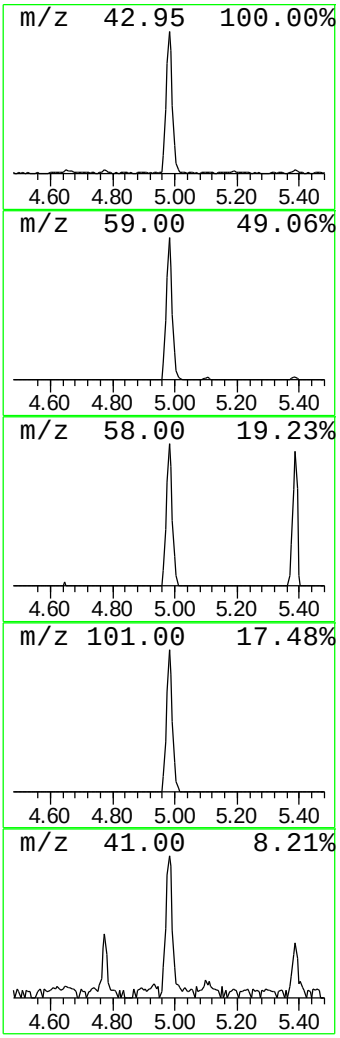
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	6.39 ng	273769	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	36
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Acetone	58	C3H6O	000067-64-1	9
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9





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Data File : BF097688.D
Acq On : 15 Aug 2017 13:53
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

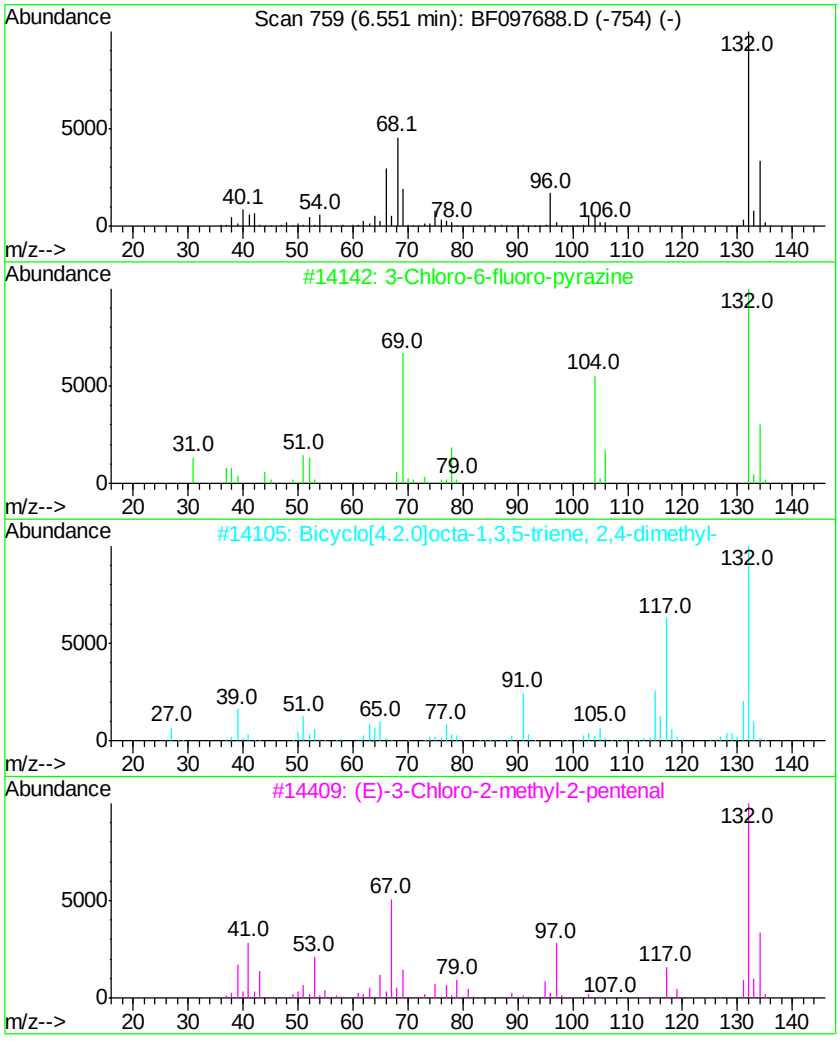
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

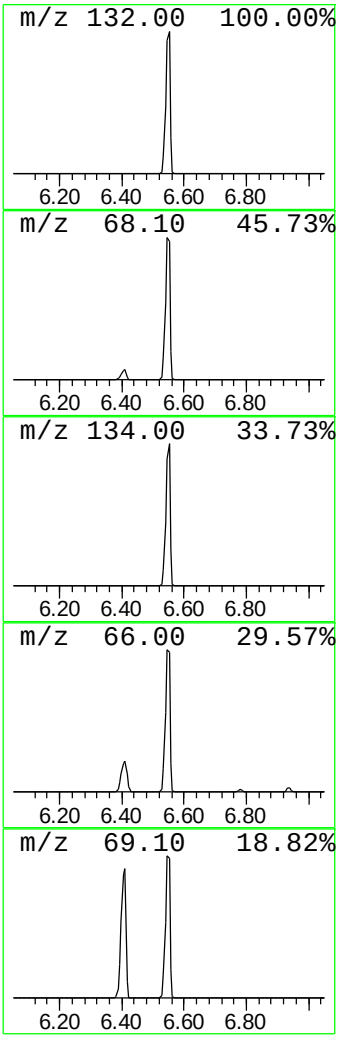
****

Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	60.90 ng	2607380	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097688.D
Acq On : 15 Aug 2017 13:53
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

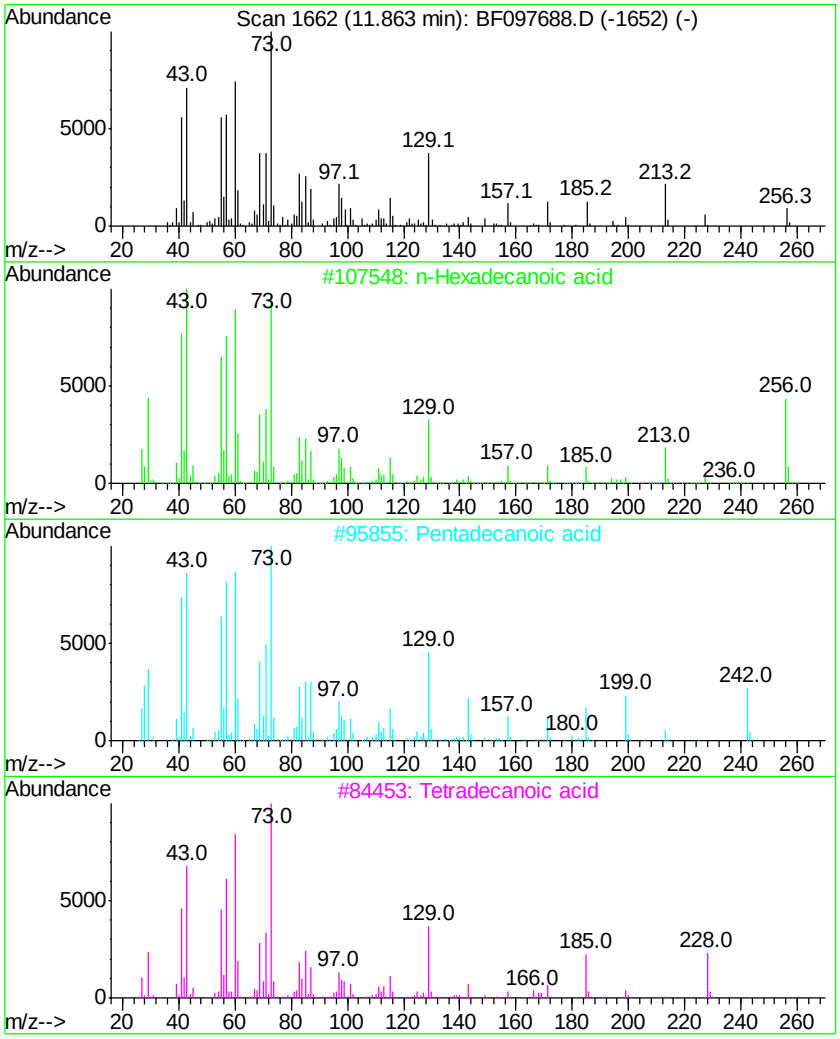
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

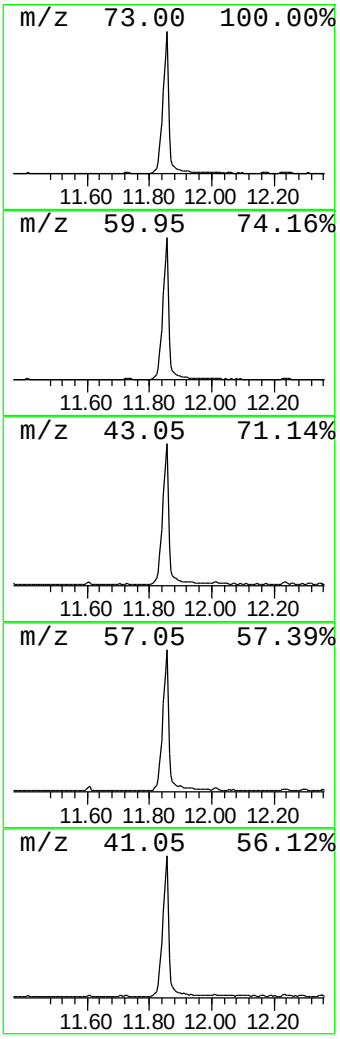
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	53.84 ng	2787620	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20
5	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097688.D
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Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

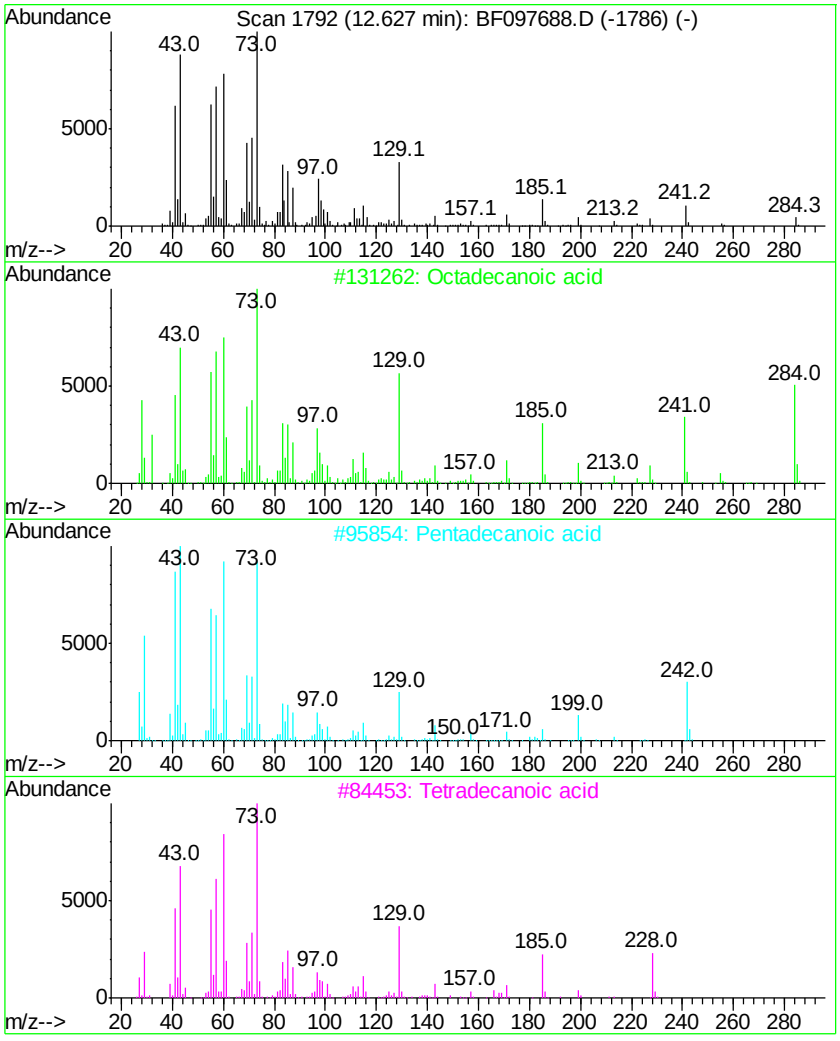
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

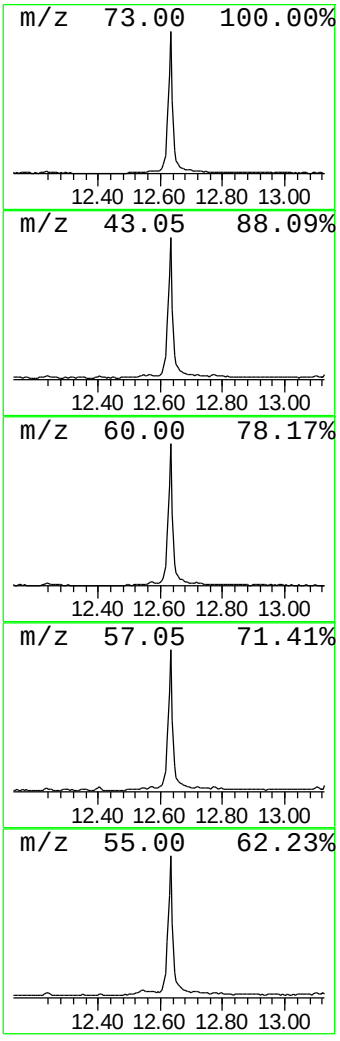
****

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	45.83 ng	2059790	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25





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Sample : I4705-01
Misc :
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Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
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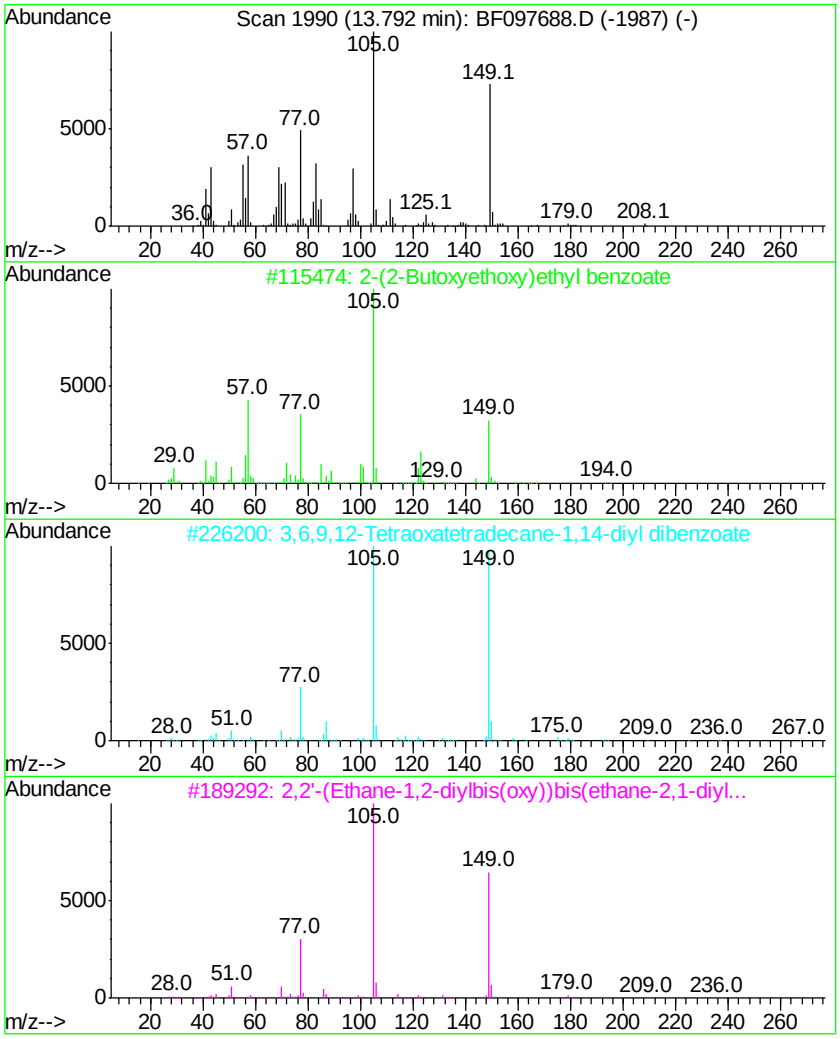
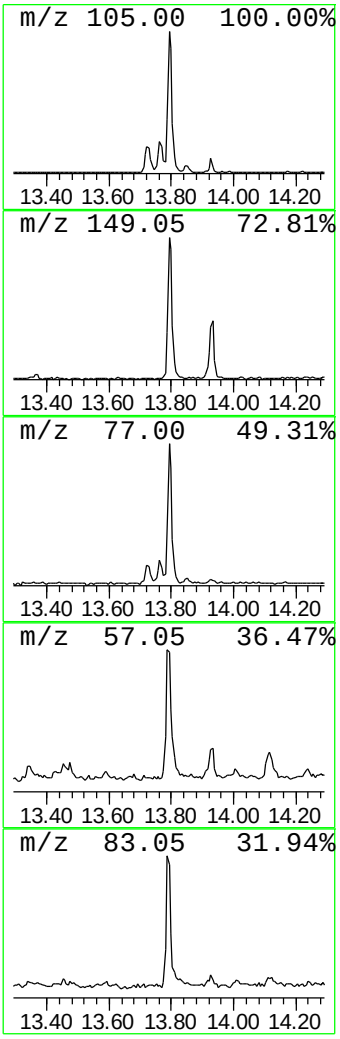
Peak Number 6 unknown13.79 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	7.85 ng	352814	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Butoxyethoxy)ethyl benzoate	266	C15H22O4	1000366-98-4	35
2	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	27
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	27
4	Malonic acid, 2-butyl octadecyl ...	412	C25H48O4	1000349-08-4	22
5	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	14





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Misc :
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Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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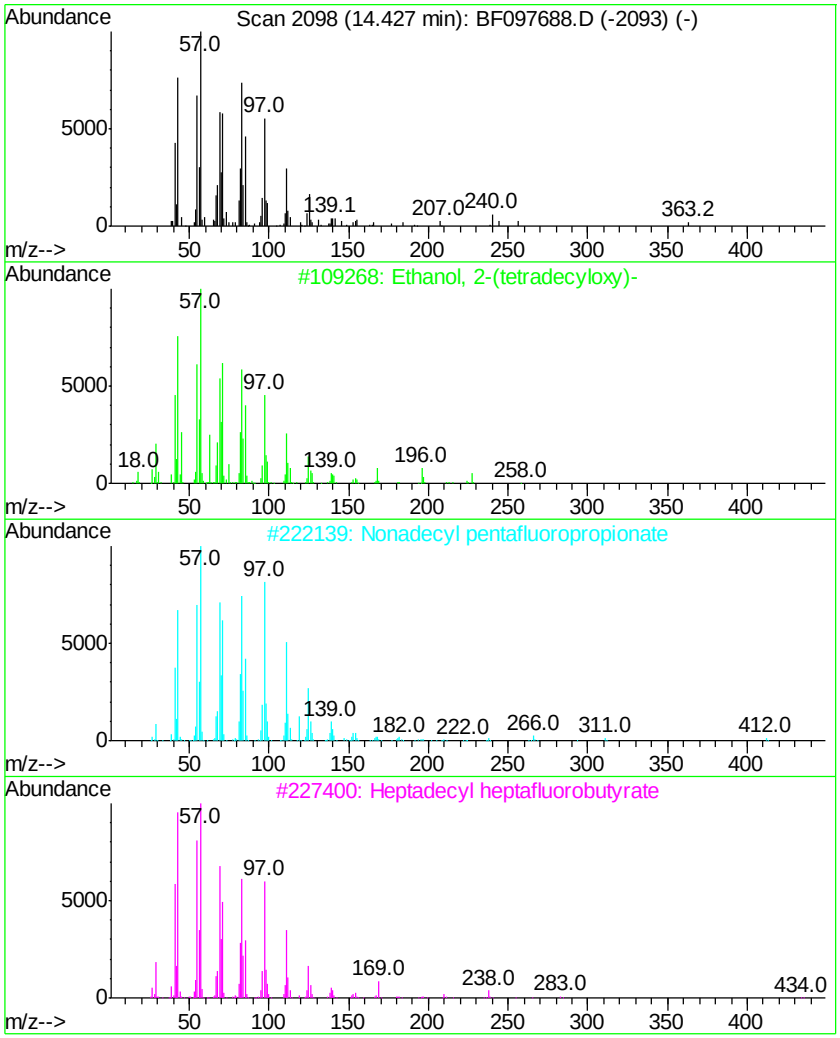
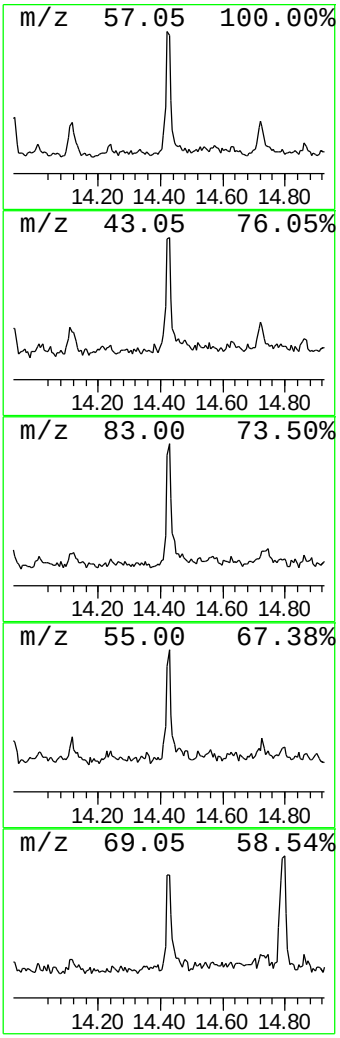
Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	3.62 ng	162877	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	81
5	1-Heptacosanol	396	C27H56O	002004-39-9	81





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Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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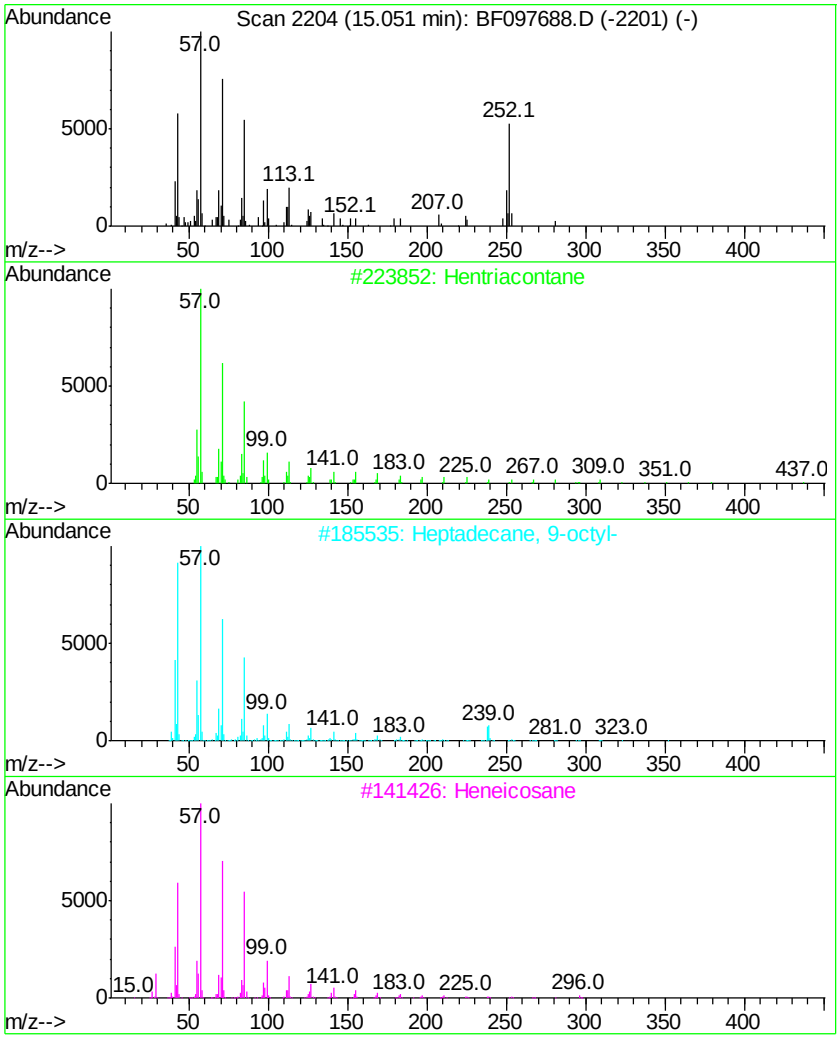
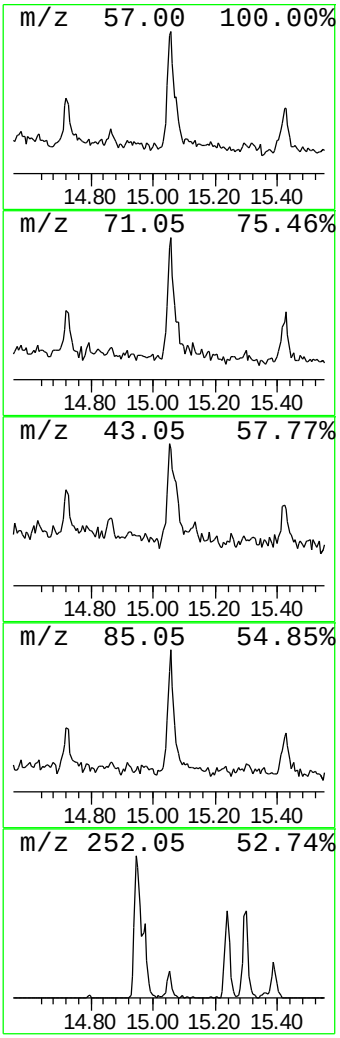
Peak Number 9 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	2.67 ng	100567	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	58
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	53
3	Heneicosane	296	C21H44	000629-94-7	52
4	2-methyloctacosane	408	C29H60	1000376-72-8	49
5	Tetratetracontane	619	C44H90	007098-22-8	49





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097688.D
Acq On : 15 Aug 2017 13:53
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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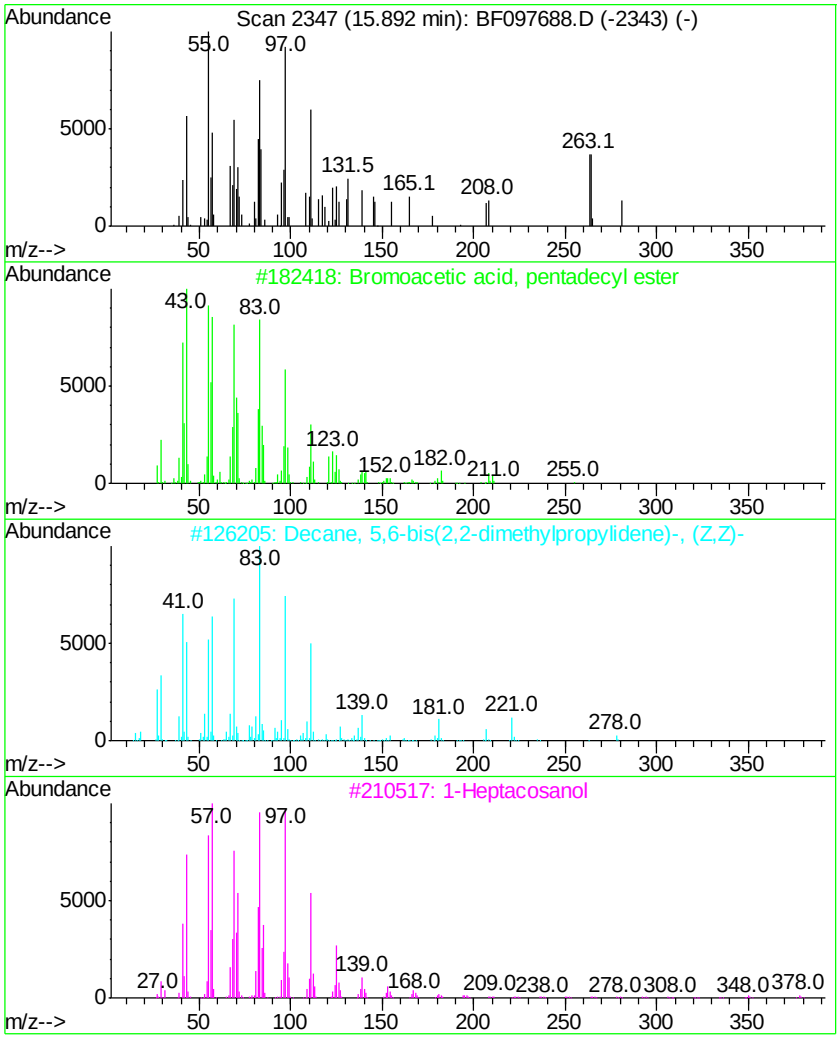
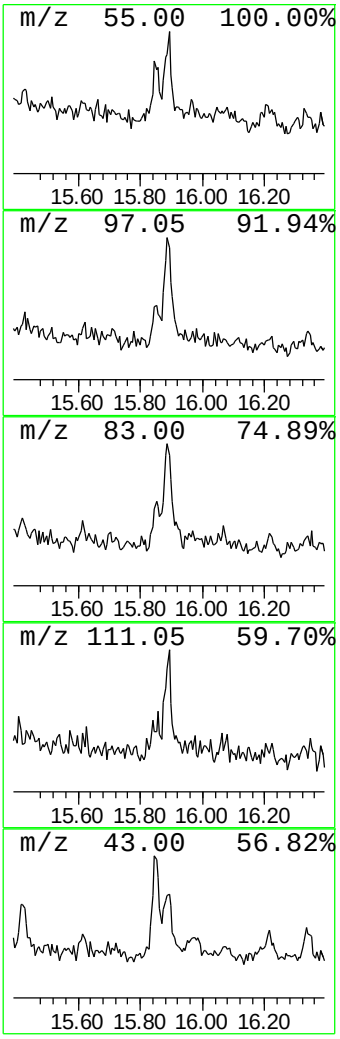
Peak Number 10 Bromoacetic acid, pentadecy... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	2.27 ng	85675	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	50
2	Decane, 5,6-bis(2,2-dimethylprop...	278	C20H38	073002-85-4	47
3	1-Heptacosanol	396	C27H56O	002004-39-9	46
4	1-Eicosanol	298	C20H42O	000629-96-9	43
5	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	38





Library Search Compound Report

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Data File : BF097688.D
Acq On : 15 Aug 2017 13:53
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

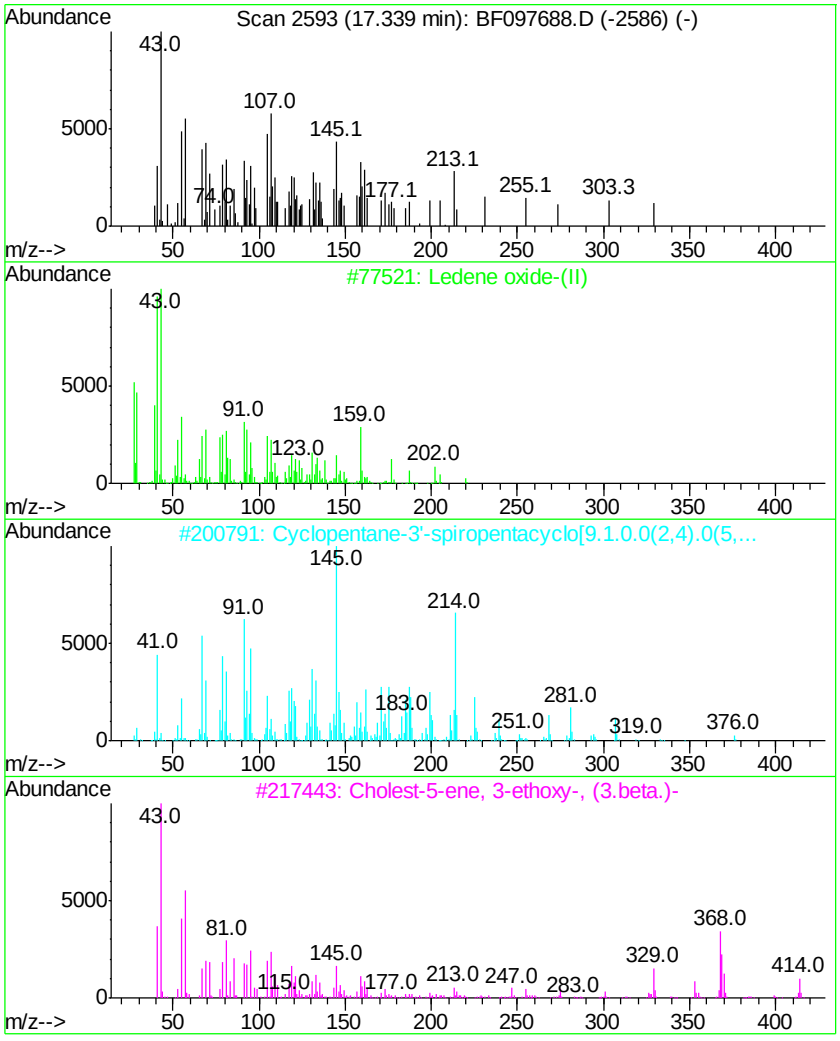
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

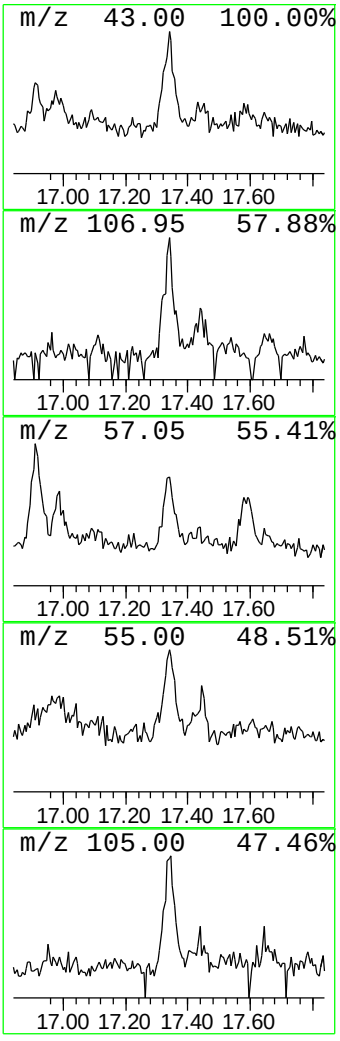
****

Peak Number 11 unknown17.34 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.34	3.82 ng	144096	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ledene oxide-(II)	220	C15H24O	1000159-36-7	32
2	Cyclopentane-3'-spiropentacyclo[...	376	C28H40	1000150-19-8	27
3	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	25
4	Benzimidazole, 2-ethyl-1-propyl-	188	C12H16N2	024103-02-4	22
5	Allopregnane-3.beta.,7.alpha.-di...	334	C21H34O3	000566-20-1	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097688.D
Acq On : 15 Aug 2017 13:53
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

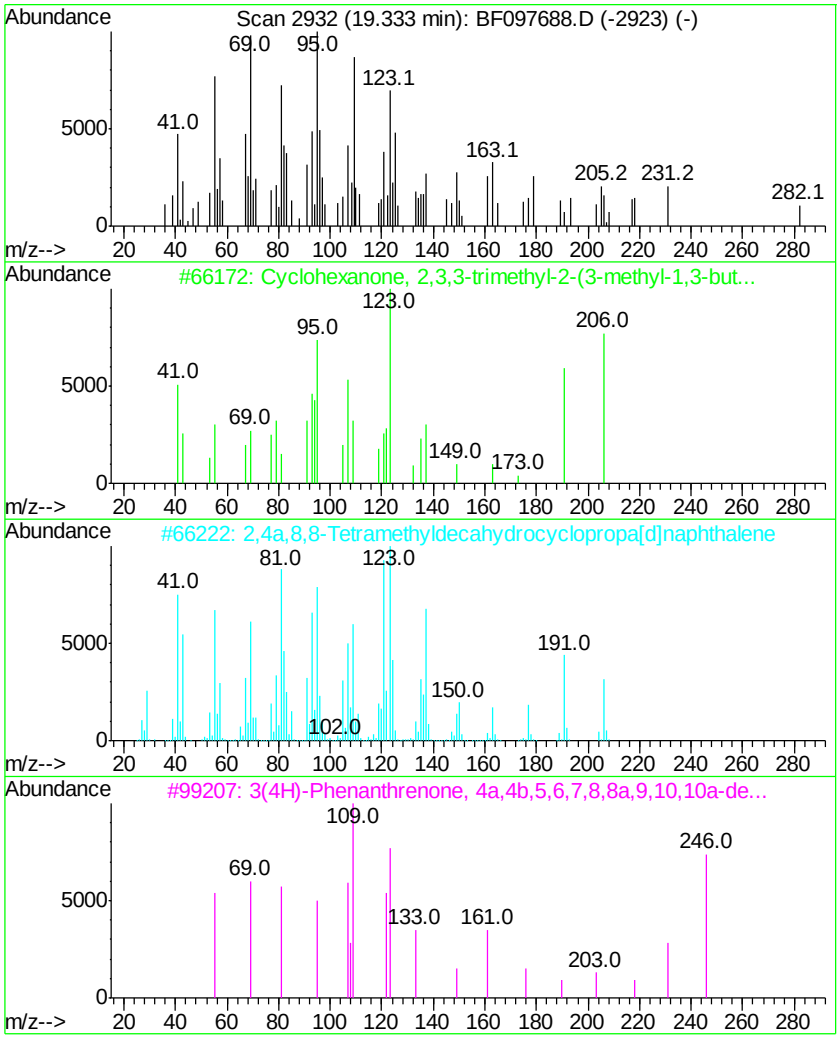
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

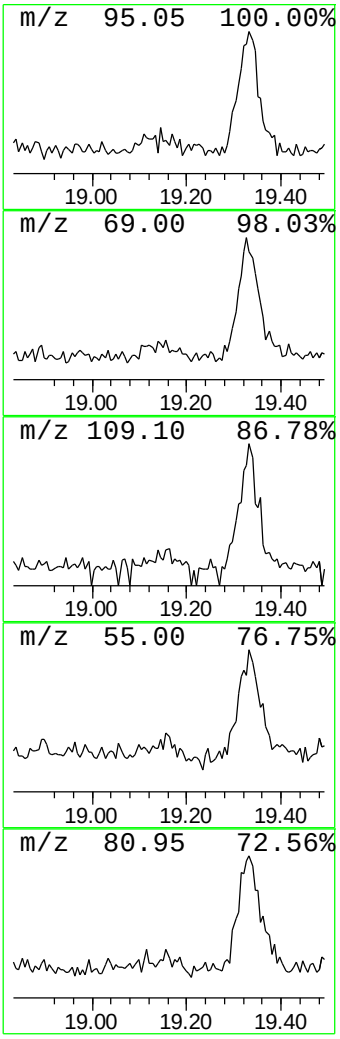
****

Peak Number 12 Cyclohexanone, 2,3,3-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	4.89 ng	184311	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-91-9	51
2	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	43
3	3(4H)-Phenanthrenone, 4a,4b,5,6,...	246	C17H26O	057684-12-5	30
4	Caparratriene	206	C15H26	1000374-08-7	30
5	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097688.D
Acq On : 15 Aug 2017 13:53
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
2-Pentanone, 4-hy...	4.98	6.4	ng	273769	1	6.78	856257	20.0
unknown6.55	6.55	60.9	ng	2607380	1	6.78	856257	20.0
n-Hexadecanoic acid	11.86	53.8	ng	2787620	4	11.30	1035530	20.0
Octadecanoic acid	12.63	45.8	ng	2059790	5	13.93	898957	20.0
unknown13.79	13.79	7.8	ng	352814	5	13.93	898957	20.0
Ethanol, 2-(tetra...	14.43	3.6	ng	162877	5	13.93	898957	20.0
Hentriacontane	15.05	2.7	ng	100567	6	15.36	753532	20.0
Bromoacetic acid,...	15.89	2.3	ng	85675	6	15.36	753532	20.0
unknown17.34	17.34	3.8	ng	144096	6	15.36	753532	20.0
Cyclohexanone, 2,...	19.33	4.9	ng	184311	6	15.36	753532	20.0