LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098770.D
Acq On : 24 Sep 2017 6:55
Operator : SJ/JU
Sample : I5298-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.240	21	26	32	rVB	277991	352624	12.14%	1.591%
2	5.146	517	520	527	rVB	197066	194842	6.71%	0.879%
3	5.534	582	586	590	rBV	1200557	1100607	37.90%	4.966%
4	6.534	752	756	759	rBV	836197	654276	22.53%	2.952%
5	6.563	759	761	768	rVB	44689	38204	1.32%	0.172%
6	6.687	778	782	785	rBV	2165619	1867875	64.32%	8.428%
7	6.922	818	822	825	rBV	1076023	834506	28.74%	3.766%
8	7.081	844	849	852	rBV	2820976	2494698	85.91%	11.257%
9	7.481	912	917	920	rBV	1881593	1860448	64.07%	8.395%
10	8.204	1036	1040	1043	rBV	1208364	949342	32.69%	4.284%
11	9.275	1217	1222	1226	rBV	3011835	2903940	100.00%	13.103%
12	9.957	1334	1338	1342	rVB	951513	815450	28.08%	3.680%
13	10.745	1468	1472	1475	rBV	1110144	922975	31.78%	4.165%
14	11.445	1587	1591	1594	rBV	1011254	782382	26.94%	3.530%
15	12.145	1706	1710	1716	rVB2	40174	44408	1.53%	0.200%
16	12.839	1825	1828	1832	rBV	554464	454484	15.65%	2.051%
17	12.916	1839	1841	1845	rVB	83807	68105	2.35%	0.307%
18	13.027	1856	1860	1864	rBV	2680518	2617885	90.15%	11.813%
19	13.545	1945	1948	1952	rBV	450300	374474	12.90%	1.690%
20	13.592	1952	1956	1958	rVV	76027	77516	2.67%	0.350%
21	13.616	1958	1960	1963	rVB	40770	32038	1.10%	0.145%
22	13.816	1989	1994	2000	rBV2	24530	36245	1.25%	0.164%
23	13.921	2007	2012	2015	rBV	97612	90521	3.12%	0.408%
24	14.086	2036	2040	2043	rBV	899181	860760	29.64%	3.884%
25	14.233	2062	2065	2069	rBV	103191	97044	3.34%	0.438%
26	14.539	2114	2117	2121	rBV	107708	96654	3.33%	0.436%
27	14.857	2167	2171	2177	rBV	104538	107456	3.70%	0.485%
28	15.204	2226	2230	2236	rVB	92251	108779	3.75%	0.491%
29	15.574	2288	2293	2304	rBV	534442	785283	27.04%	3.543%
30	16.045	2368	2373	2377	rBV	79109	112833	3.89%	0.509%
31	16.562	2456	2461	2468	rVB2	79952	144751	4.98%	0.653%
32	17.180	2561	2566	2573	rBV2	52551	101609	3.50%	0.458%
33	17.686	2647	2652	2662	rVB9	40667	87123	3.00%	0.393%
34	17.904	2685	2689	2700	rVB2	38747	91657	3.16%	0.414%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098770.D
Acq On : 24 Sep 2017 6:55
Operator : SJ/JU
Sample : I5298-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091817-SIDI-F-U-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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 22161794

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
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Misc :
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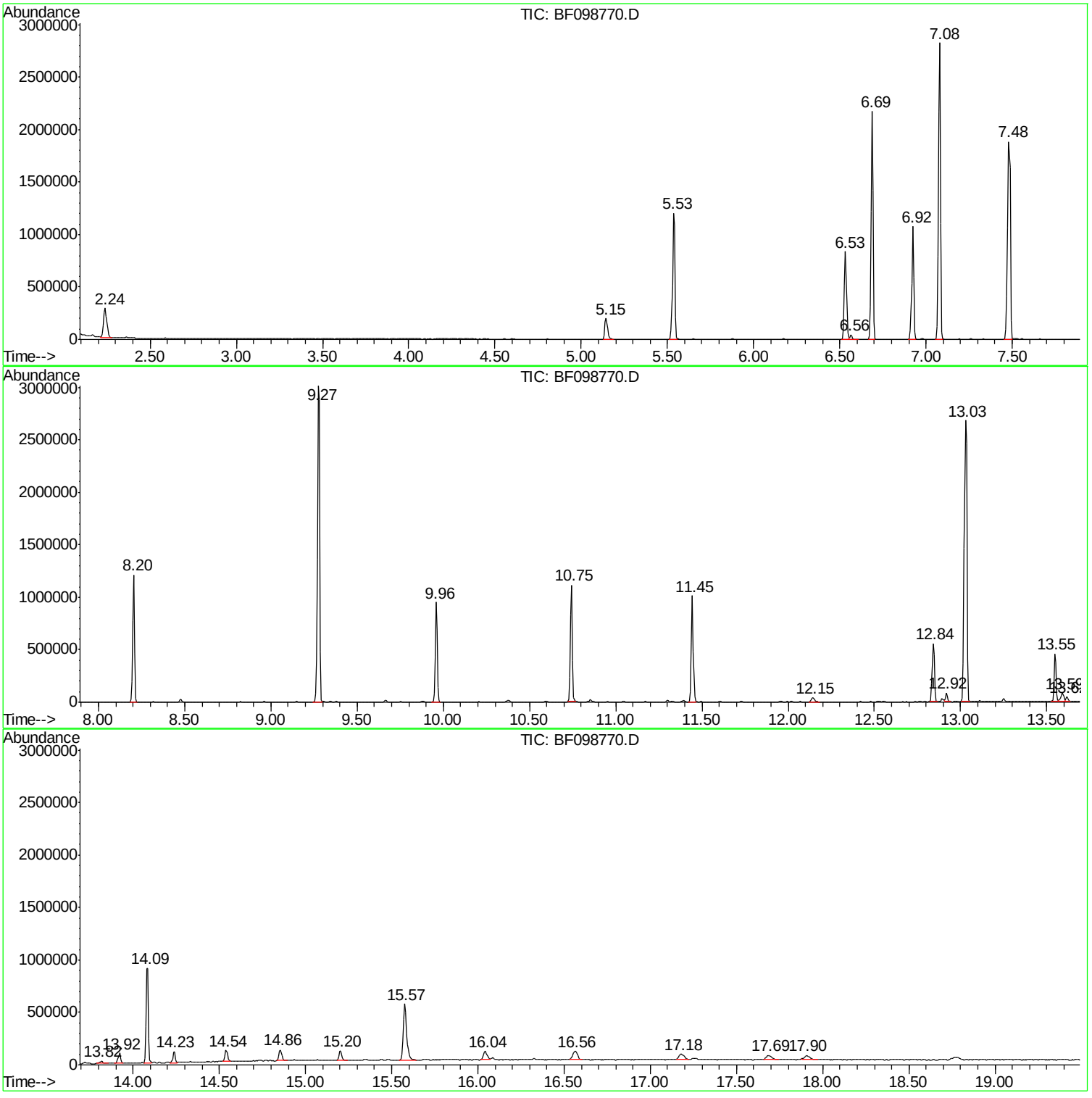
Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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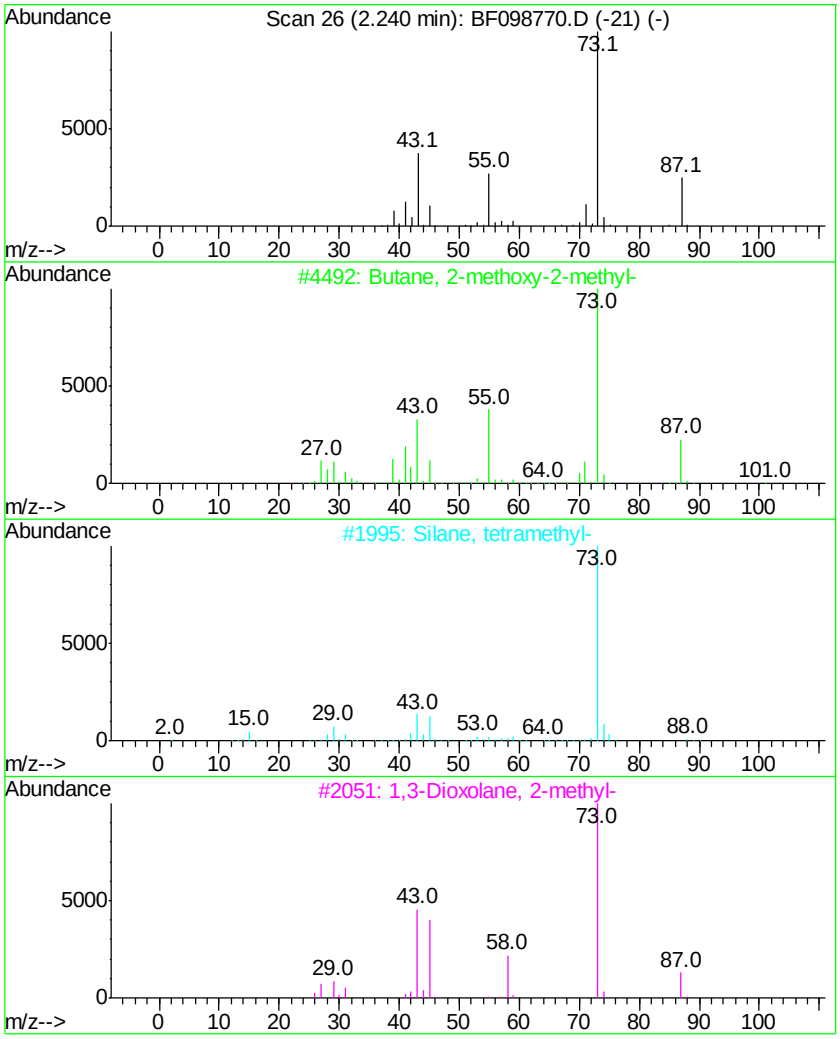
TIC Integration Parameters: LSCINT.P

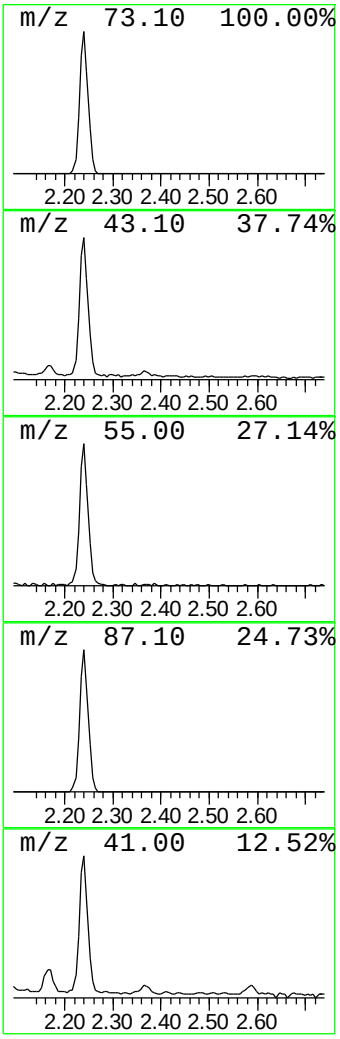
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	8.45 ng	352624	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12





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Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

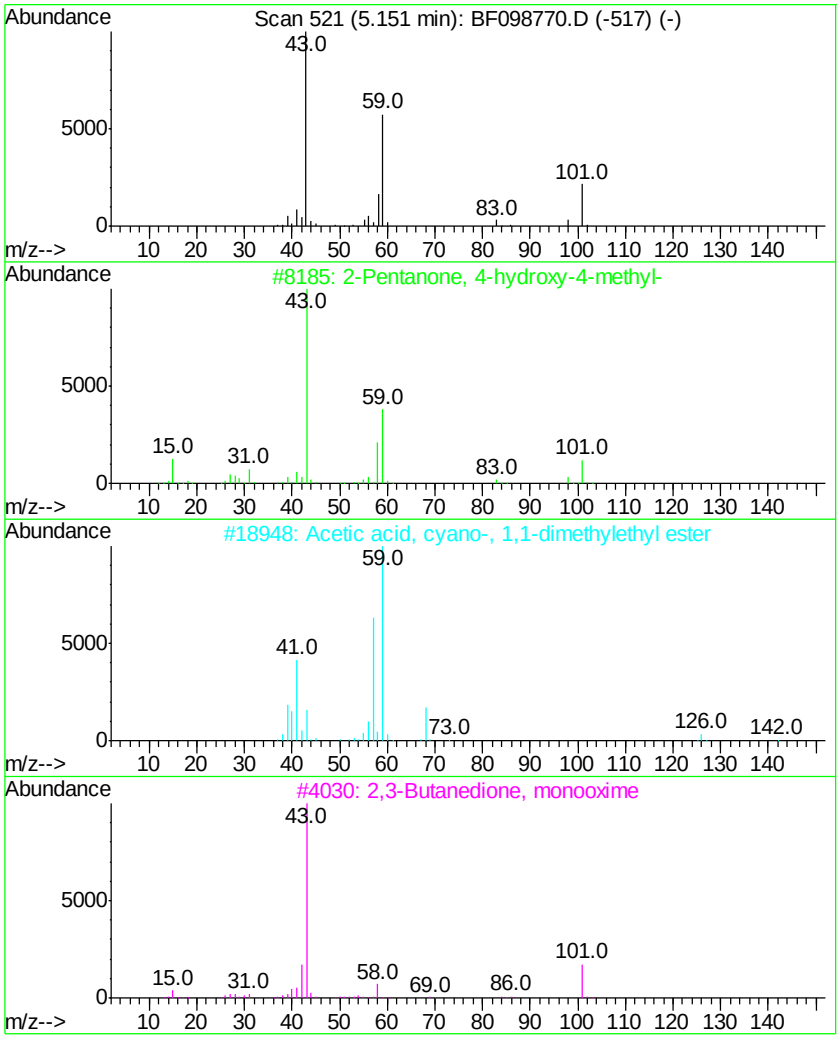
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

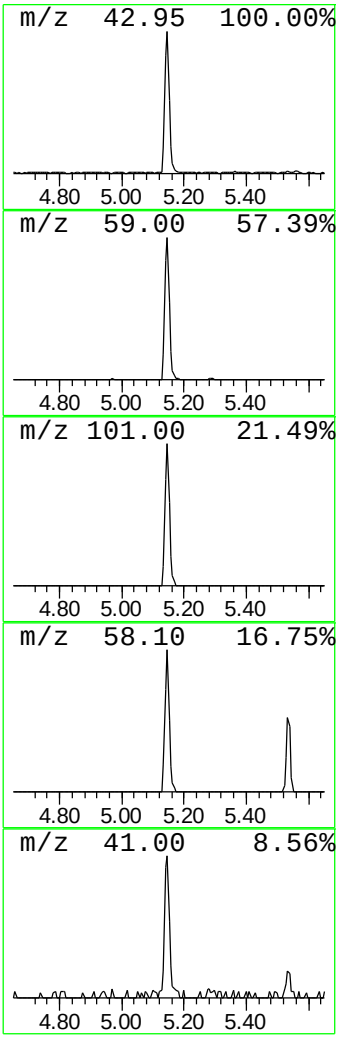
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	4.67 ng	194842	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

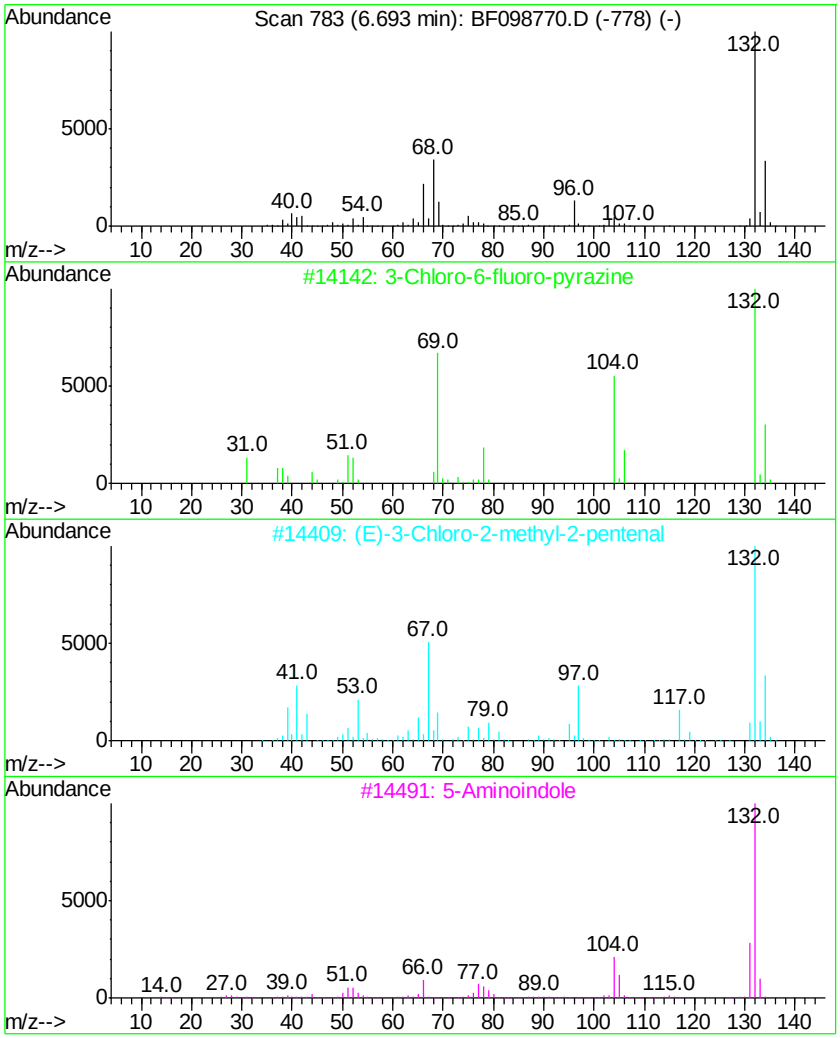
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

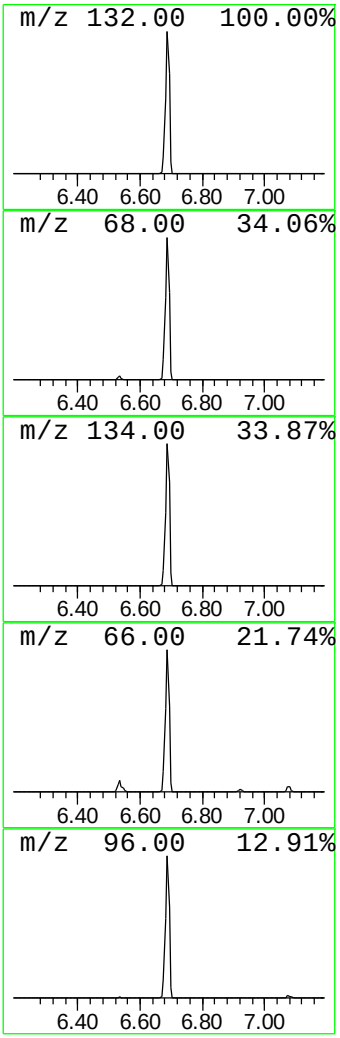
****

Peak Number 3 unknown6.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	44.77 ng	1867880	1,4-Dichlorobenzene-d4	6.92

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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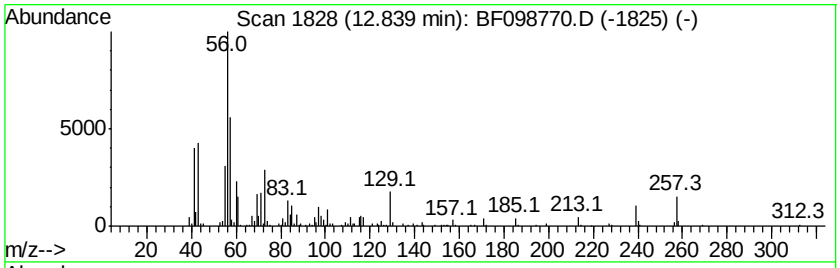
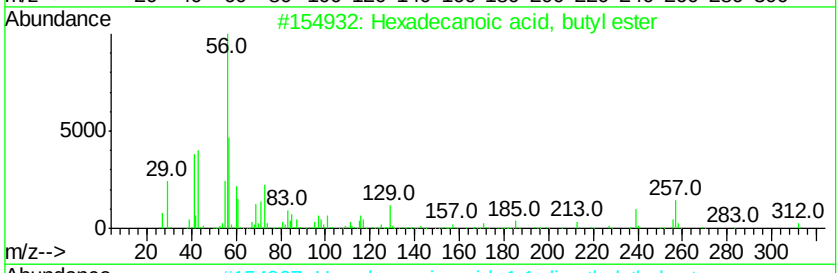
****

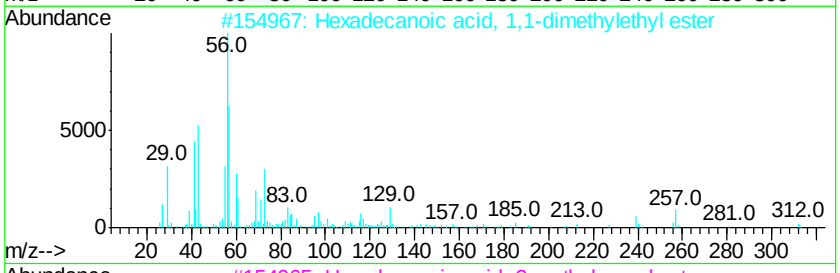
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 3

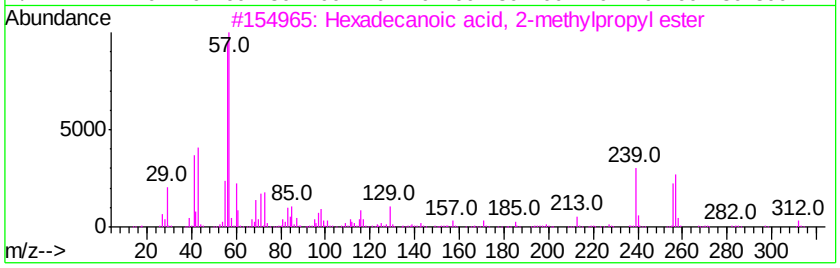
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	10.56 ng	454484	Chrysene-d12	14.09

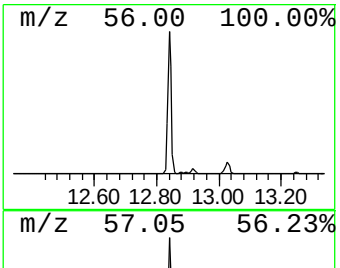
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	74
4	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38

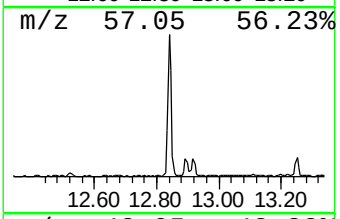


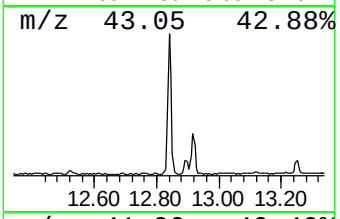


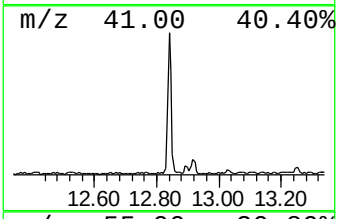


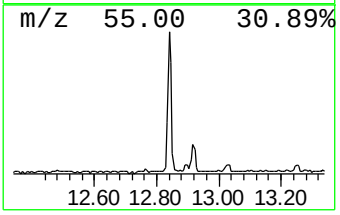












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Misc :
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Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

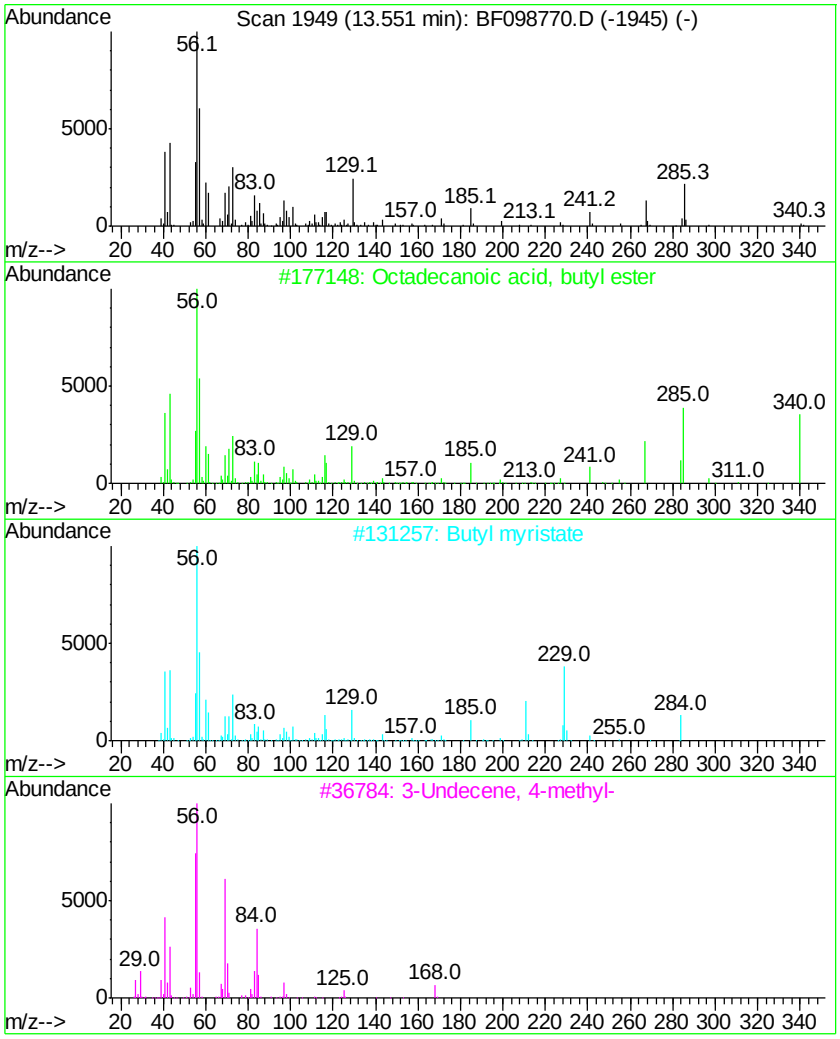
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

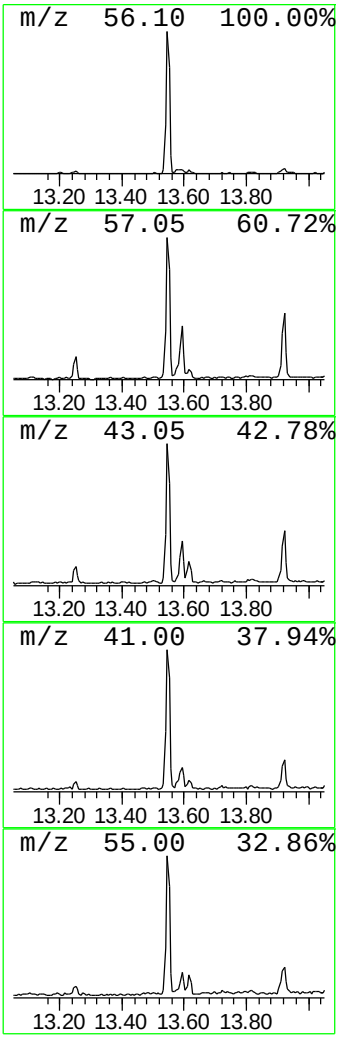
****

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	8.70 ng	374474	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Butyl myristate	284	C18H36O2	000110-36-1	64
3	3-Undecene, 4-methyl-	168	C12H24	074630-68-5	32
4	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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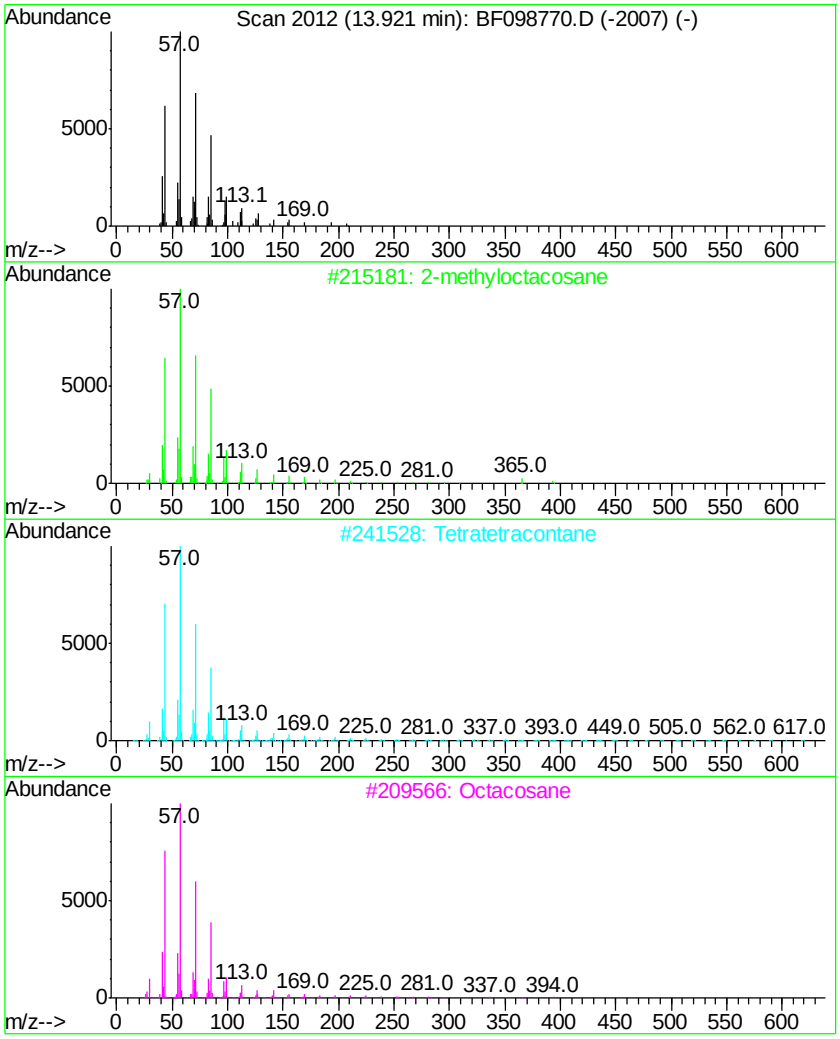
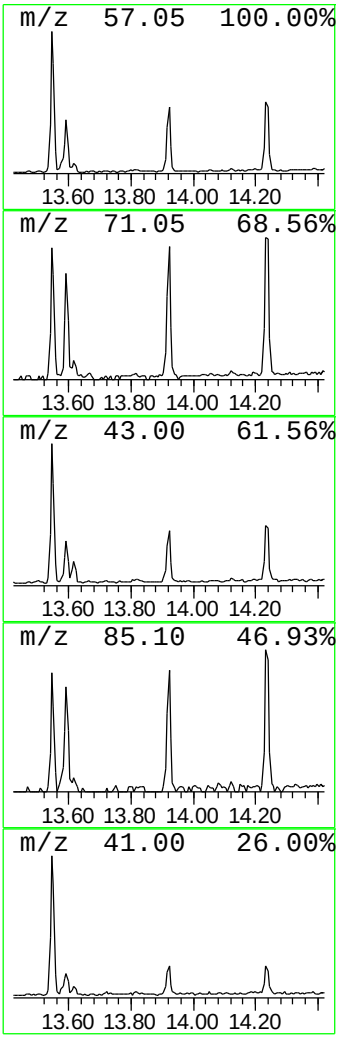
Peak Number 7 2-methyloctacosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	2.10 ng	90521	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Hexacosane	366	C26H54	000630-01-3	87





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Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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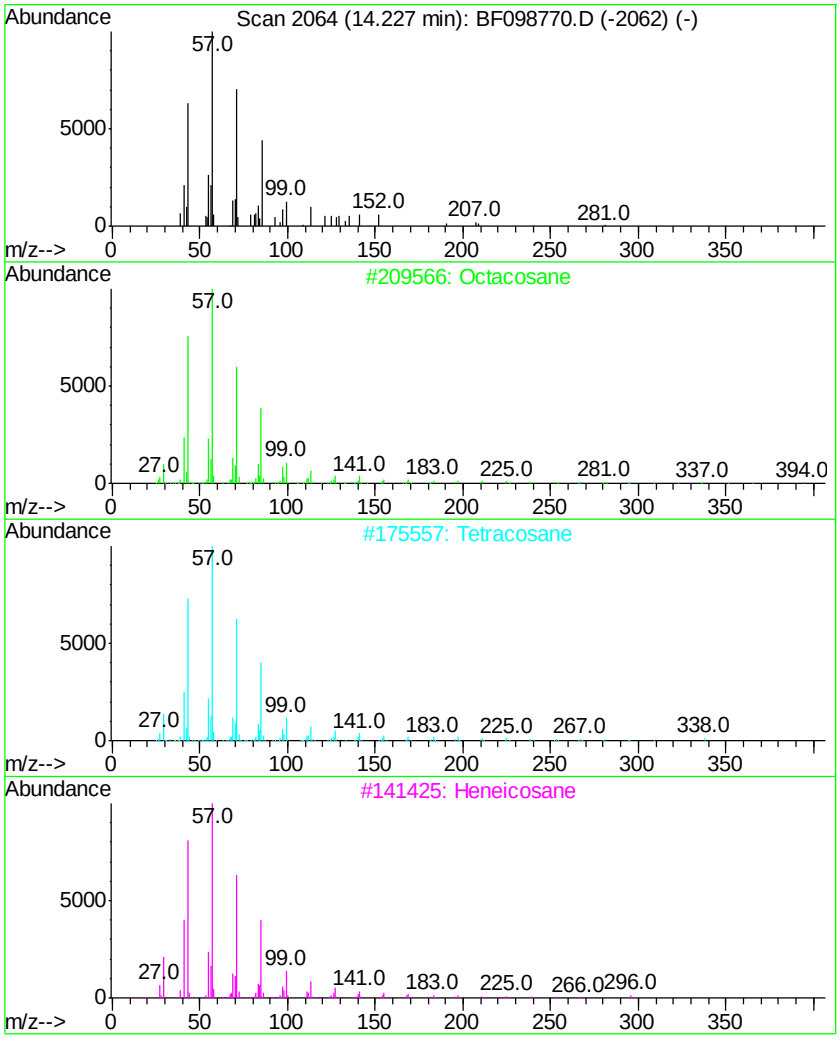
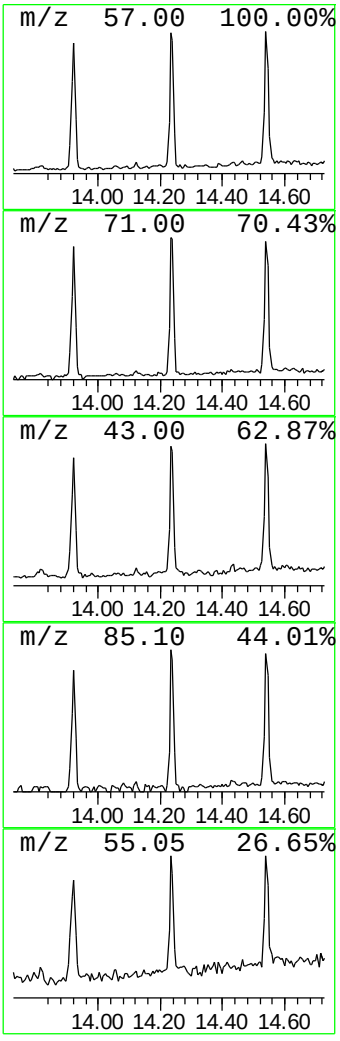
Peak Number 8 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.25 ng	97044	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	10-Methylnonadecane	282	C20H42	056862-62-5	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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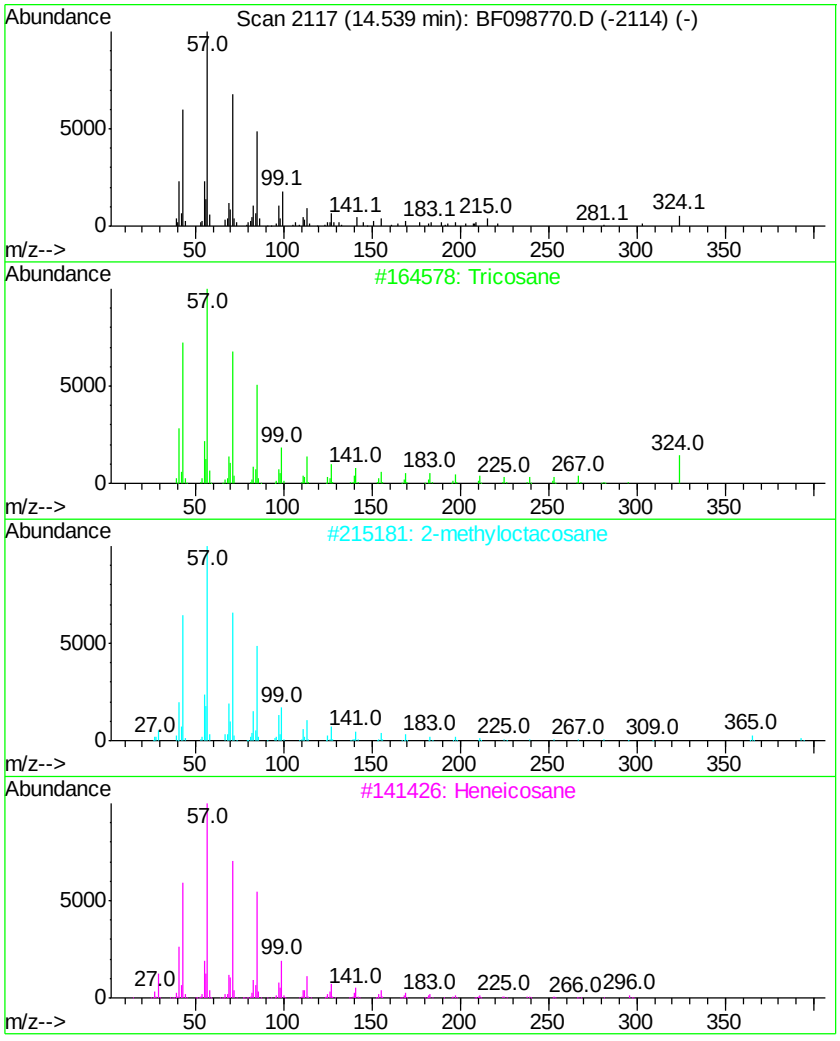
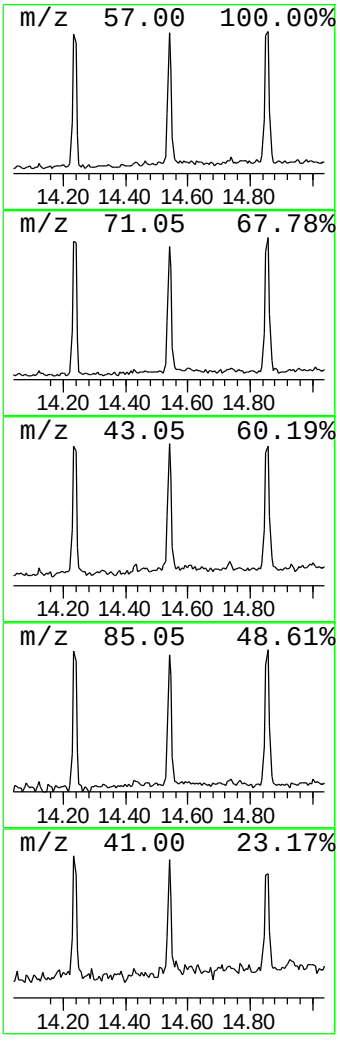
Peak Number 9 Tricosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	2.25 ng	96654	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Tetracosane	338	C24H50	000646-31-1	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098770.D
Acq On : 24 Sep 2017 6:55
Operator : SJ/JU
Sample : I5298-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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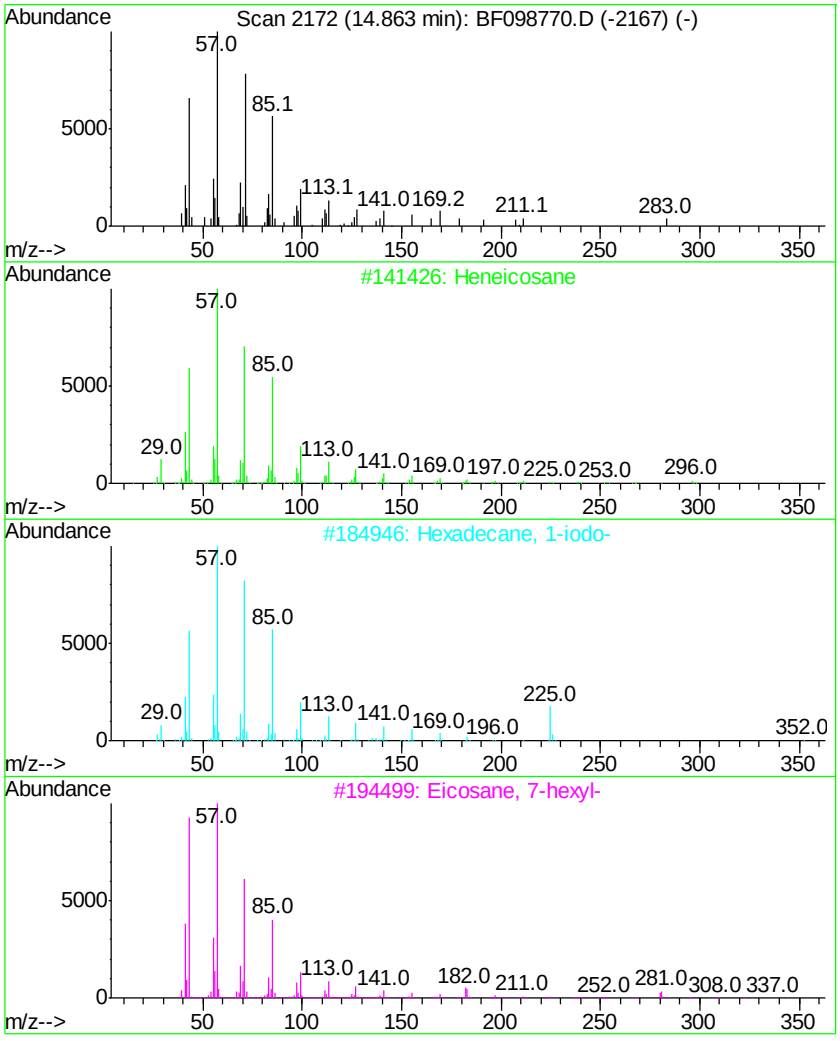
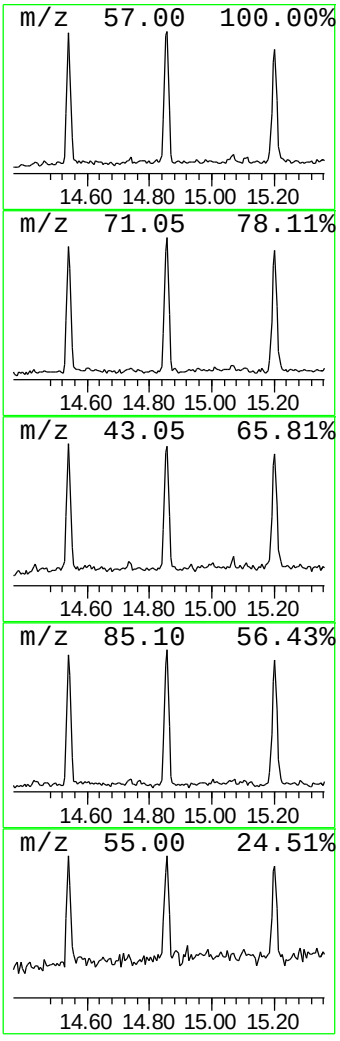
Peak Number 10 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	2.74 ng	107456	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Octacosane	394	C28H58	000630-02-4	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098770.D
Acq On : 24 Sep 2017 6:55
Operator : SJ/JU
Sample : I5298-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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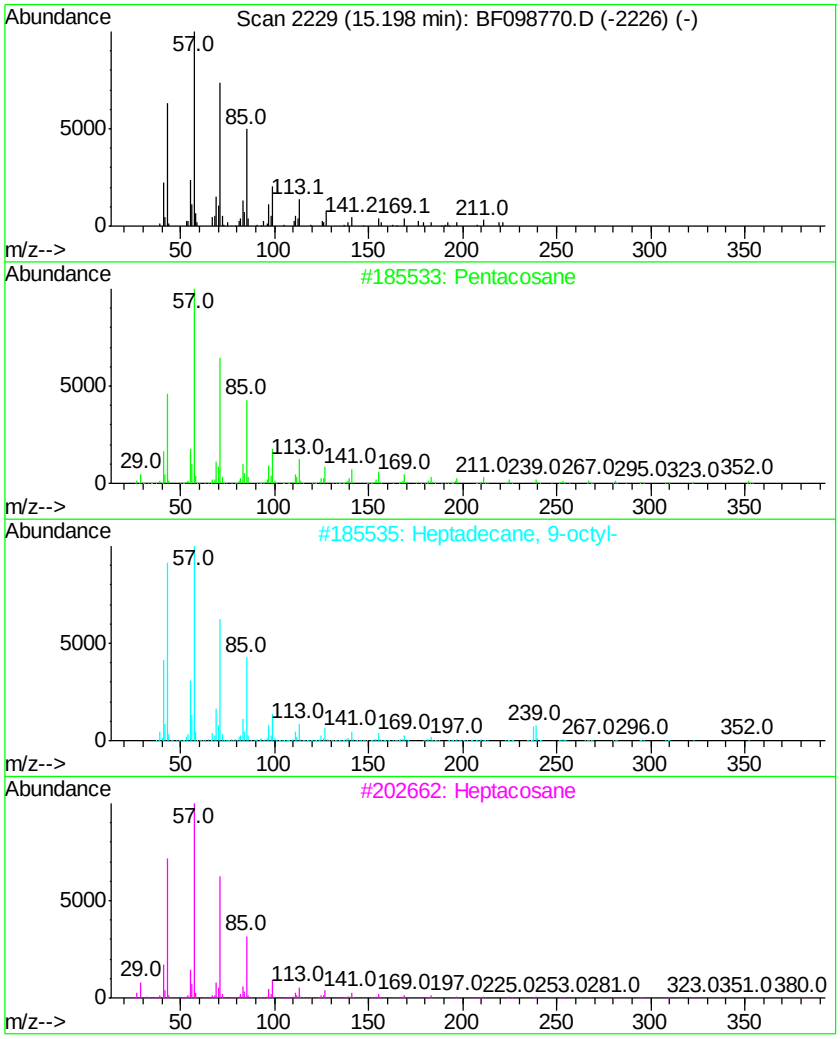
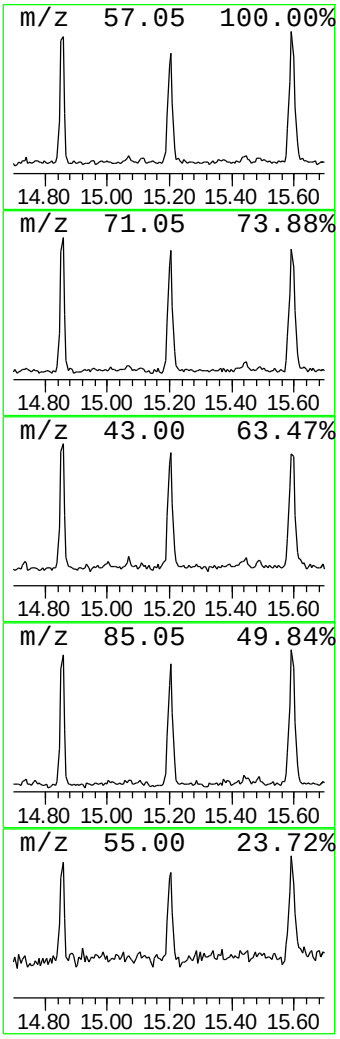
Peak Number 11 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	2.77 ng	108779	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Triacontane	422	C30H62	000638-68-6	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098770.D
Acq On : 24 Sep 2017 6:55
Operator : SJ/JU
Sample : I5298-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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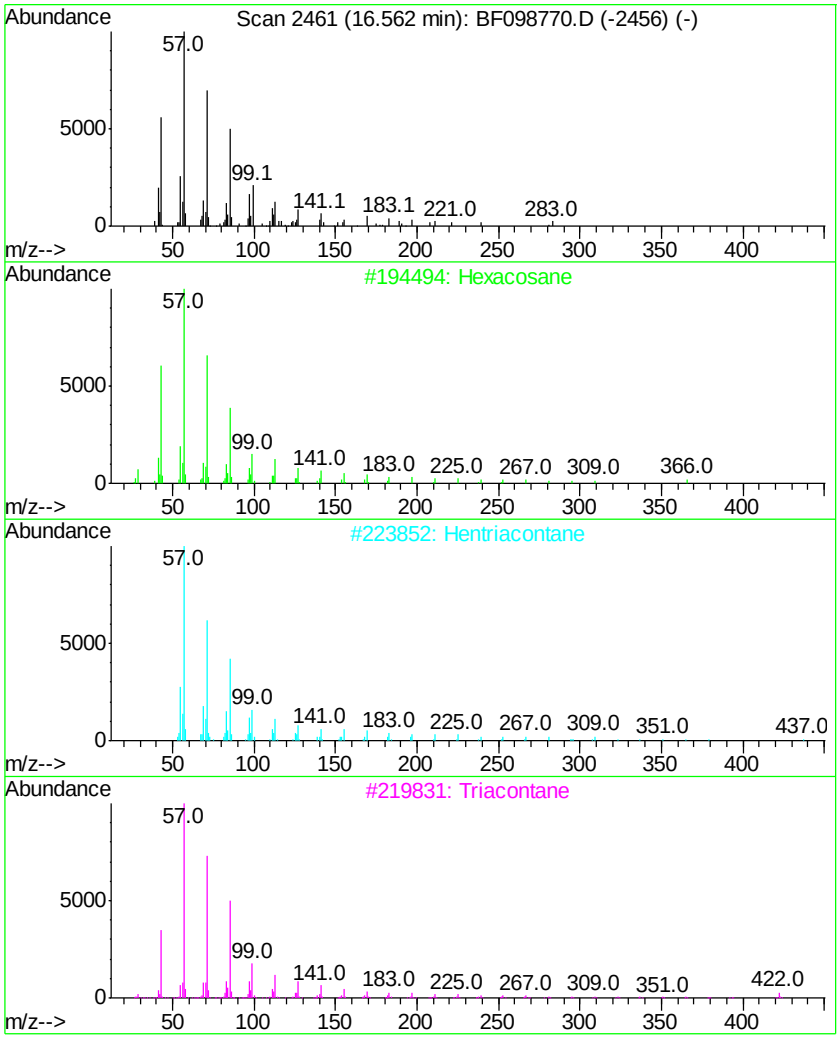
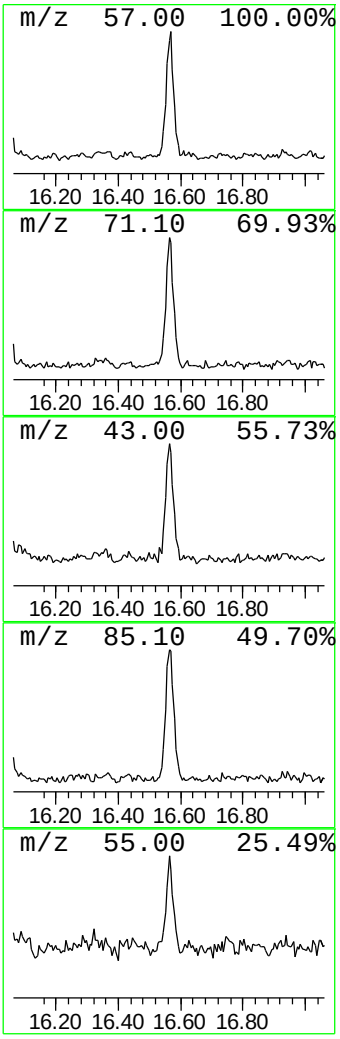
Peak Number 13 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	3.69 ng	144751	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Octacosane	394	C28H58	000630-02-4	90
5	Pentacosane	352	C25H52	000629-99-2	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098770.D
Acq On : 24 Sep 2017 6:55
Operator : SJ/JU
Sample : I5298-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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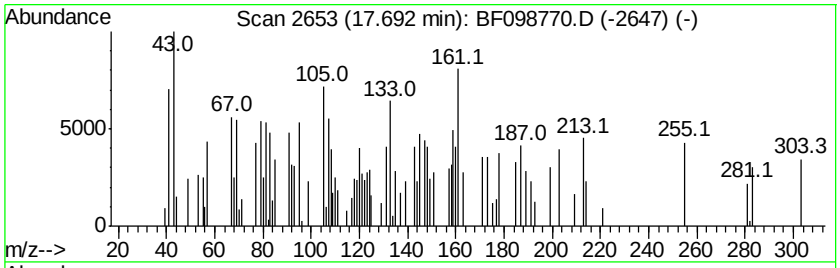
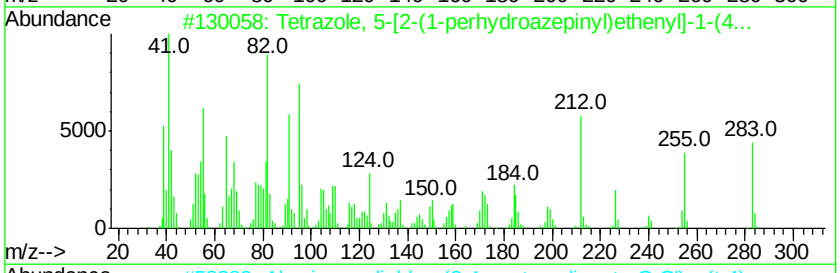
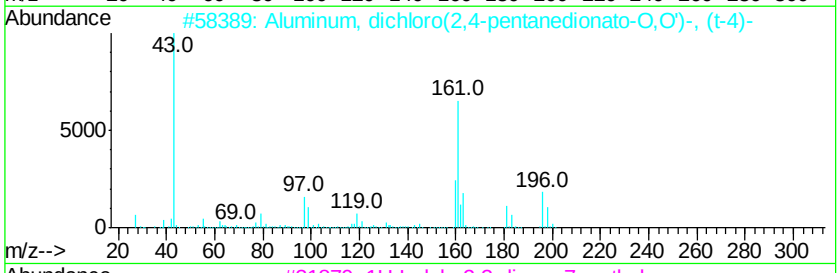
Peak Number 15 unknown17.69 Concentration Rank 15

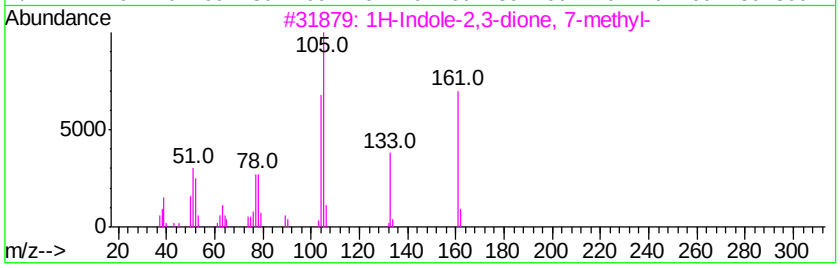
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.69	2.22 ng	87123	Perylene-d12	15.57

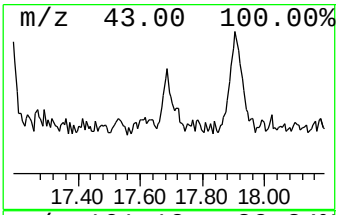
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrazole, 5-[2-(1-perhydroazepi...	283	C16H21N5	299461-62-4	11
2	Aluminum, dichloro(2,4-pentanedi...	196	C5H7AlCl2O2	015488-12-7	10
3	1H-Indole-2,3-dione, 7-methyl-	161	C9H7NO2	001127-59-9	10
4	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	10
5	4,5-di-epi-aristolochene	204	C15H24	1000374-17-1	9

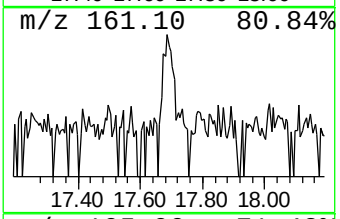


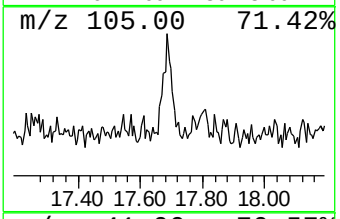


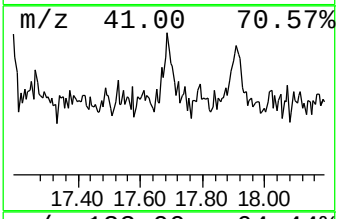


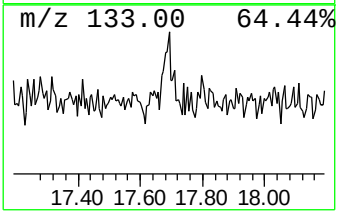












Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098770.D
Acq On : 24 Sep 2017 6:55
Operator : SJ/JU
Sample : I5298-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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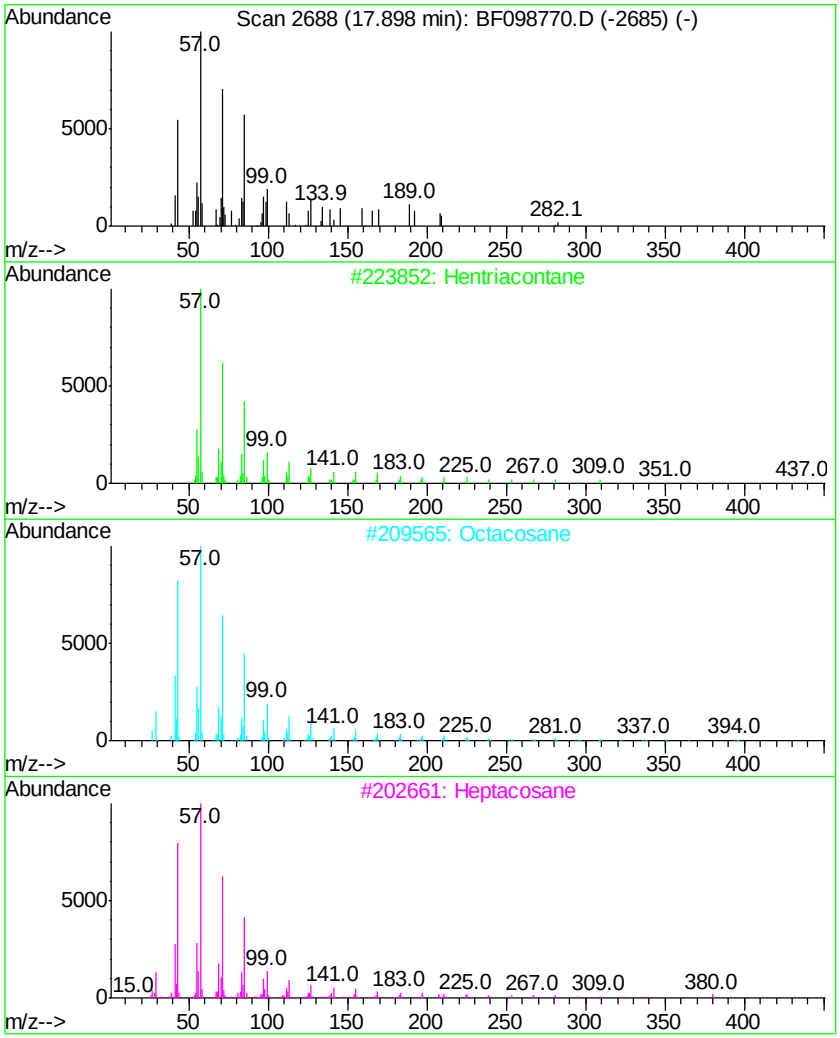
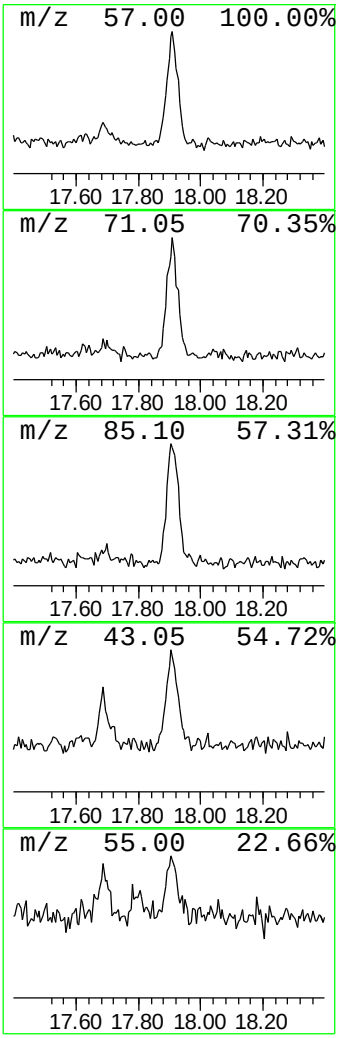
Peak Number 16 Hentriacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	2.33 ng	91657	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	87
2	Octacosane	394	C28H58	000630-02-4	80
3	Heptacosane	380	C27H56	000593-49-7	80
4	Hexacosane	366	C26H54	000630-01-3	74
5	Eicosane	282	C20H42	000112-95-8	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092317\
Data File : BF098770.D
Acq On : 24 Sep 2017 6:55
Operator : SJ/JU
Sample : I5298-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091817-SIDI-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	2.24	8.4	ng	352624	1	6.92	834506	20.0
2-Pentanone, 4-hy...	5.15	4.7	ng	194842	1	6.92	834506	20.0
unknown6.69	6.69	44.8	ng	1867880	1	6.92	834506	20.0
Hexadecanoic acid...	12.84	10.6	ng	454484	5	14.09	860760	20.0
Octadecanoic acid...	13.55	8.7	ng	374474	5	14.09	860760	20.0
2-methyloctacosane	13.92	2.1	ng	90521	5	14.09	860760	20.0
Octacosane	14.23	2.3	ng	97044	5	14.09	860760	20.0
Tricosane	14.54	2.3	ng	96654	5	14.09	860760	20.0
Heneicosane	14.86	2.7	ng	107456	6	15.57	785283	20.0
Pentacosane	15.20	2.8	ng	108779	6	15.57	785283	20.0
Hexacosane	16.56	3.7	ng	144751	6	15.57	785283	20.0
unknown17.69	17.69	2.2	ng	87123	6	15.57	785283	20.0
Hentriacontane	17.90	2.3	ng	91657	6	15.57	785283	20.0