LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102992.D
Acq On : 14 Feb 2018 16:30
Operator : SJ/JU
Sample : J1539-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MAIN-ST-LINE-3-EW@4.5

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-BF020318.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	2.151	6	11	22	rVB	724959	994577	25.01%	2.913%
2	5.110	510	514	526	rVB	106745	149957	3.77%	0.439%
3	5.498	575	580	583	rBV	3738126	3692823	92.87%	10.817%
4	6.504	746	751	764	rVB2	3186394	3976496	100.00%	11.648%
5	6.645	770	775	778	rBV	3782601	3650891	91.81%	10.694%
6	6.704	782	785	789	rVB3	44274	43351	1.09%	0.127%
7	6.875	810	814	818	rBV	1307209	1047127	26.33%	3.067%
8	7.033	837	841	844	rBV	3040761	2628408	66.10%	7.699%
9	7.439	905	910	913	rBV	2488973	2310351	58.10%	6.767%
10	7.510	919	922	928	rVB3	36907	43214	1.09%	0.127%
11	8.157	1029	1032	1035	rBV	1574711	1316366	33.10%	3.856%
12	8.739	1128	1131	1135	rVB	63700	51078	1.28%	0.150%
13	8.869	1150	1153	1157	rBV	74852	59714	1.50%	0.175%
14	8.969	1167	1170	1174	rBV	50040	41763	1.05%	0.122%
15	9.233	1210	1215	1218	rBV	3531579	3166628	79.63%	9.275%
16	9.304	1224	1227	1230	rBV	150219	113295	2.85%	0.332%
17	9.498	1256	1260	1265	rBV	34883	50928	1.28%	0.149%
18	9.569	1268	1272	1275	rBV4	44084	56647	1.42%	0.166%
19	9.622	1278	1281	1284	rBV	351934	272206	6.85%	0.797%
20	9.833	1310	1317	1321	rBV	258652	213528	5.37%	0.625%
21	9.910	1327	1330	1334	rBV	1288478	1206498	30.34%	3.534%
22	10.063	1352	1356	1359	rBV4	28756	40986	1.03%	0.120%
23	10.116	1362	1365	1369	rVB3	41216	53023	1.33%	0.155%
24	10.157	1369	1372	1376	rBV3	57394	64633	1.63%	0.189%
25	10.310	1395	1398	1399	rBV	43906	41004	1.03%	0.120%
26	10.333	1399	1402	1405	rVB	272714	215960	5.43%	0.633%
27	10.551	1435	1439	1446	rVB	73650	94425	2.37%	0.277%
28	10.704	1461	1465	1468	rBV	1526222	1497297	37.65%	4.386%
29	10.804	1479	1482	1491	rVB	201778	290675	7.31%	0.851%
30	10.957	1504	1508	1512	rBV	47698	53338	1.34%	0.156%
31	11.257	1555	1559	1561	rBV	121550	117835	2.96%	0.345%
32	11.286	1561	1564	1570	rVB2	58749	81346	2.05%	0.238%
33	11.398	1579	1583	1586	rBV	1072388	964603	24.26%	2.825%
34	11.421	1586	1587	1593	rVB2	154845	135078	3.40%	0.396%

LSC Area Percent Report

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Operator : SJ/JU
Sample : J1539-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MAIN-ST-LINE-3-EW@4.5

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.680	1628	1631	1637	rVB	81418	62748	1.58%	0.184%
36	11.933	1666	1674	1676	rBV2	43134	89456	2.25%	0.262%
37	12.010	1684	1687	1690	rBV3	39863	49418	1.24%	0.145%
38	12.086	1697	1700	1703	rBV	60618	55753	1.40%	0.163%
39	12.474	1764	1766	1770	rBV2	41019	41033	1.03%	0.120%
40	12.615	1786	1790	1793	rBV	200170	182852	4.60%	0.536%
41	12.845	1823	1829	1832	rBV	213562	251485	6.32%	0.737%
42	12.986	1848	1853	1856	rBV	2115920	2086606	52.47%	6.112%
43	13.168	1881	1884	1887	rVB2	48979	49022	1.23%	0.144%
44	13.868	2000	2003	2010	rVB3	176735	214674	5.40%	0.629%
45	14.039	2028	2032	2035	rBV	970914	1019585	25.64%	2.986%
46	14.062	2035	2036	2039	rVB	105346	82944	2.09%	0.243%
47	14.786	2156	2159	2166	rBV2	174216	221313	5.57%	0.648%
48	15.086	2207	2210	2216	rVB	103489	161665	4.07%	0.474%
49	15.521	2279	2284	2293	rVB	640882	835295	21.01%	2.447%

Sum of corrected areas: 34139898

LSC Report - Integrated Chromatogram

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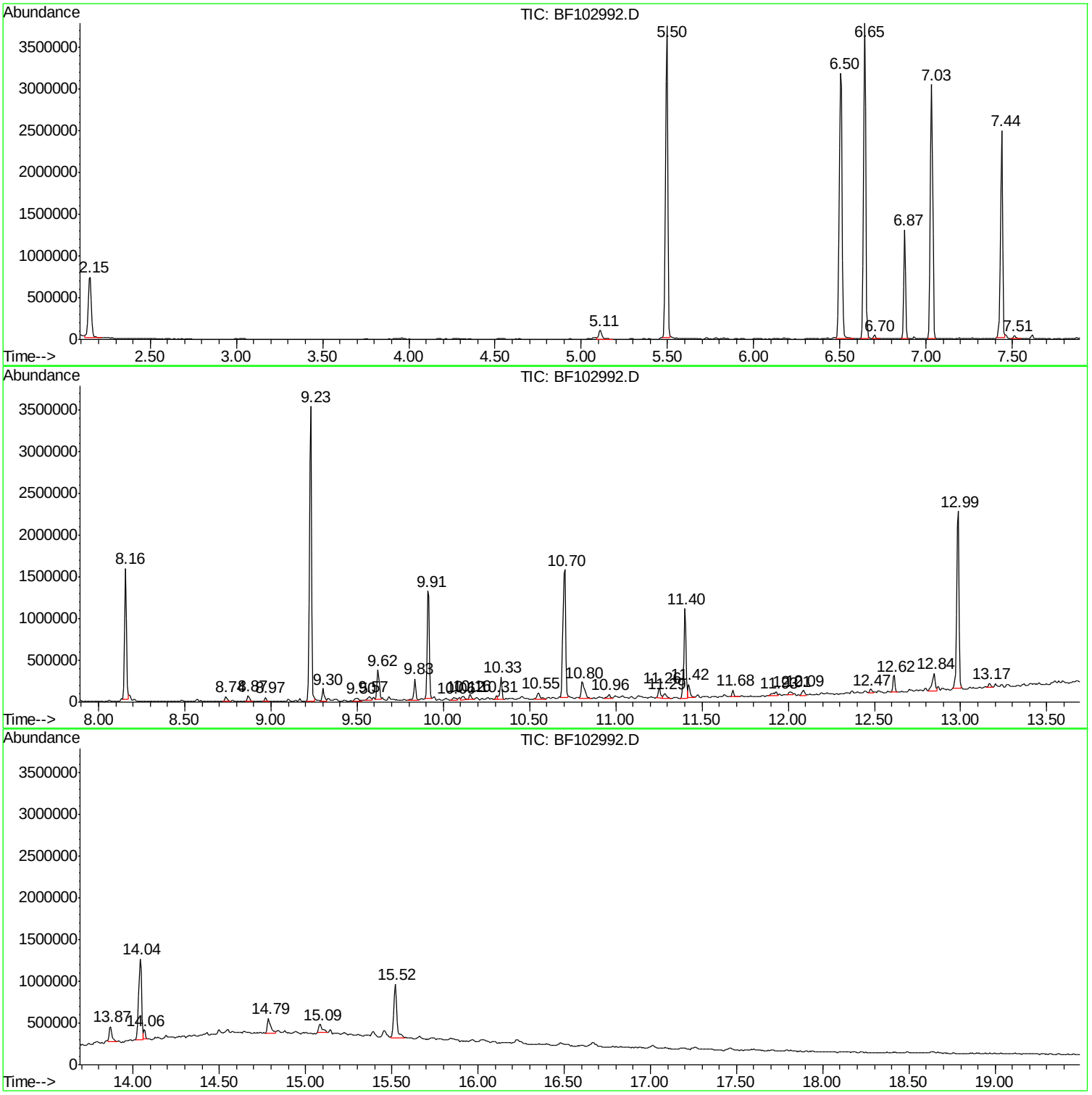
Sample : J1539-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MAIN-ST-LINE-3-EW@4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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\BF021418\
Data File : BF102992.D
Acq On : 14 Feb 2018 16:30
Operator : SJ/JU
Sample : J1539-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MAIN-ST-LINE-3-EW@4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

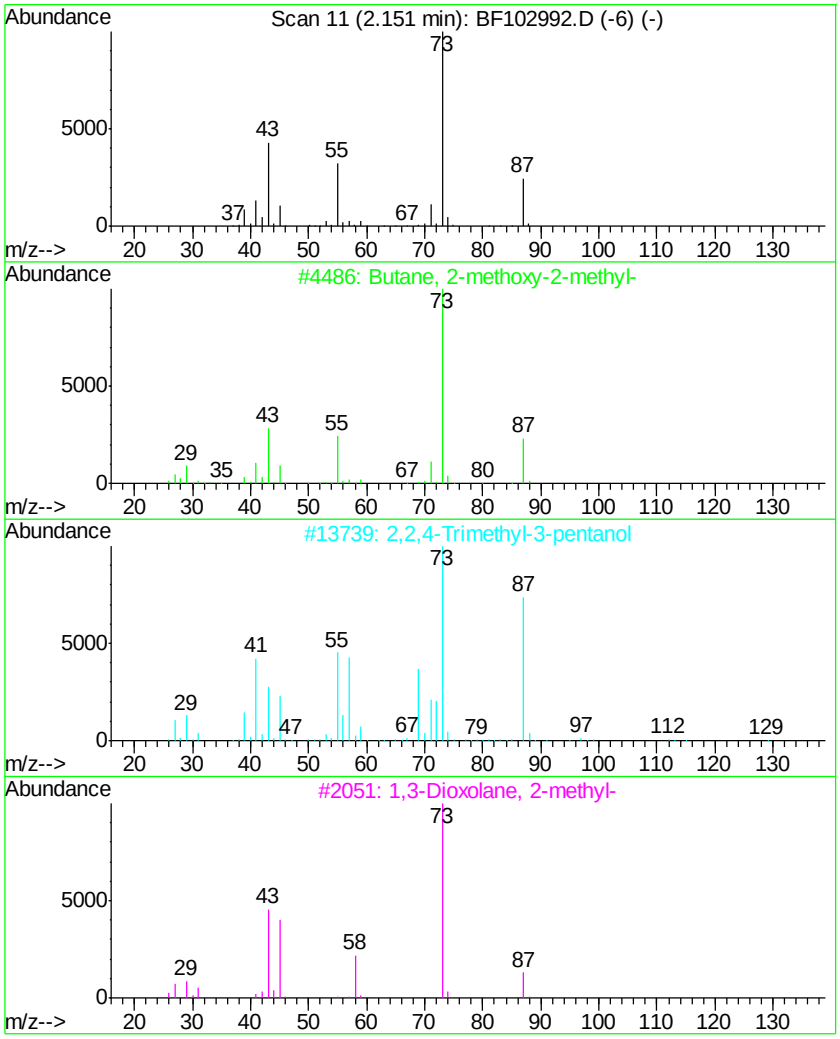
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

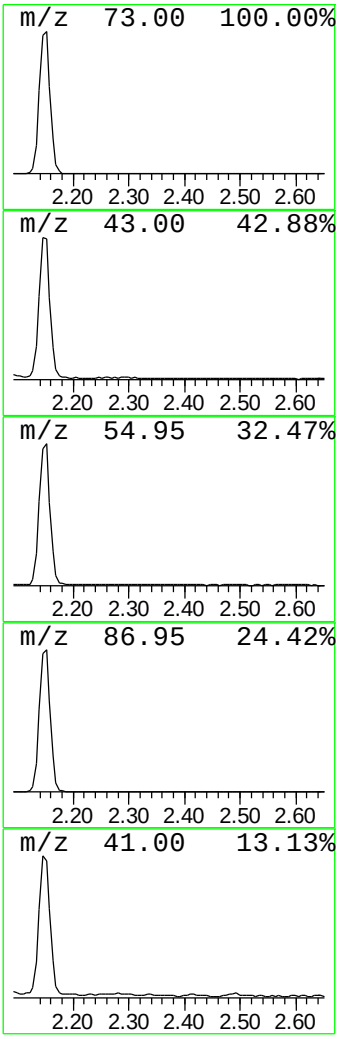
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	19.00 ng	994577	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
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Operator : SJ/JU
Sample : J1539-06
Misc :
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Instrument : BNA_F
ClientSampleId : MAIN-ST-LINE-3-EW@4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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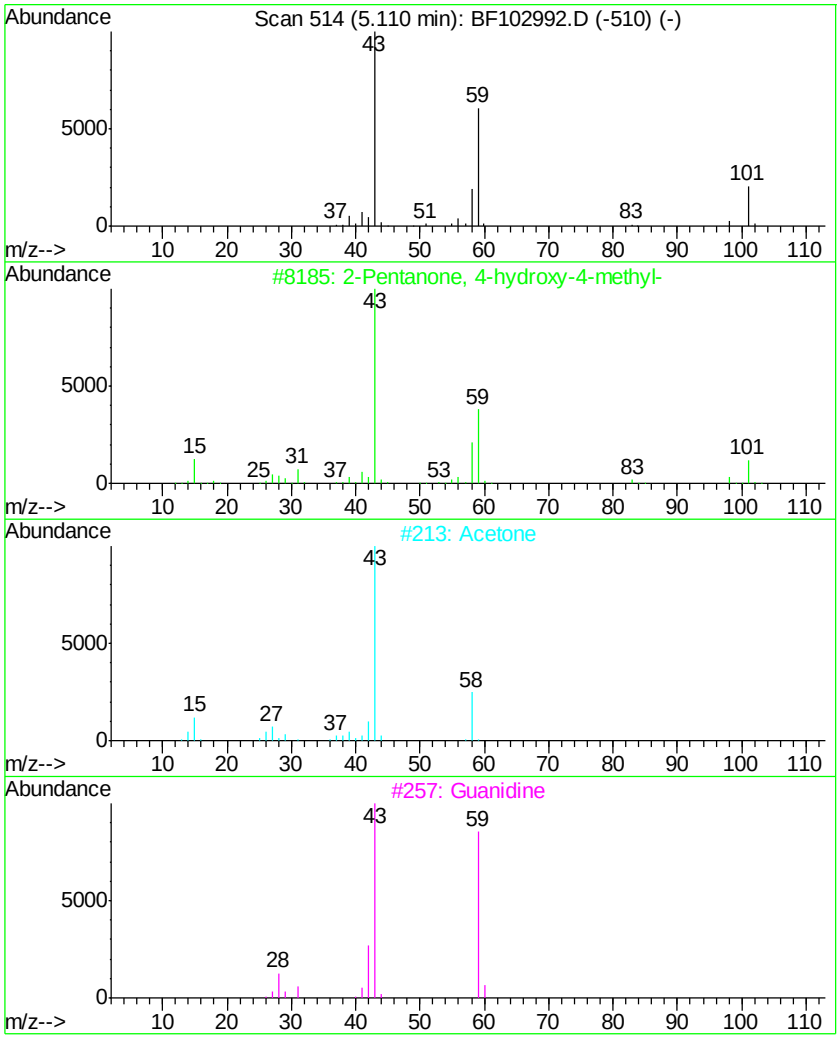
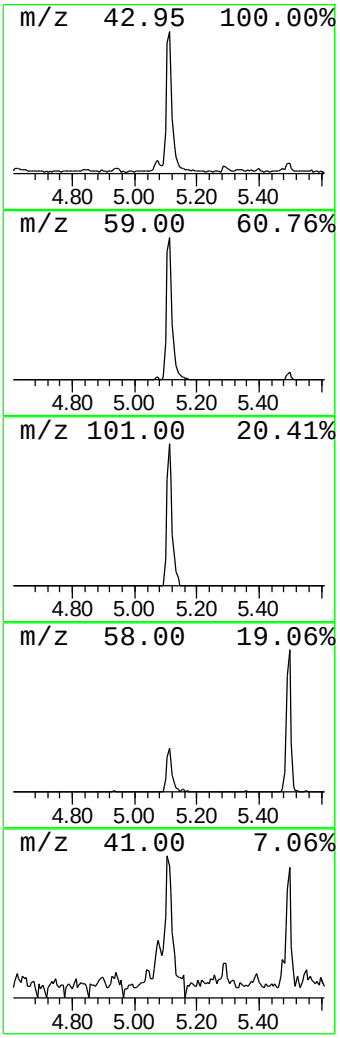
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	2.86 ng	149957	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetone	58	C3H6O	000067-64-1	9
3	Guanidine	59	CH5N3	000113-00-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102992.D
Acq On : 14 Feb 2018 16:30
Operator : SJ/JU
Sample : J1539-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MAIN-ST-LINE-3-EW@4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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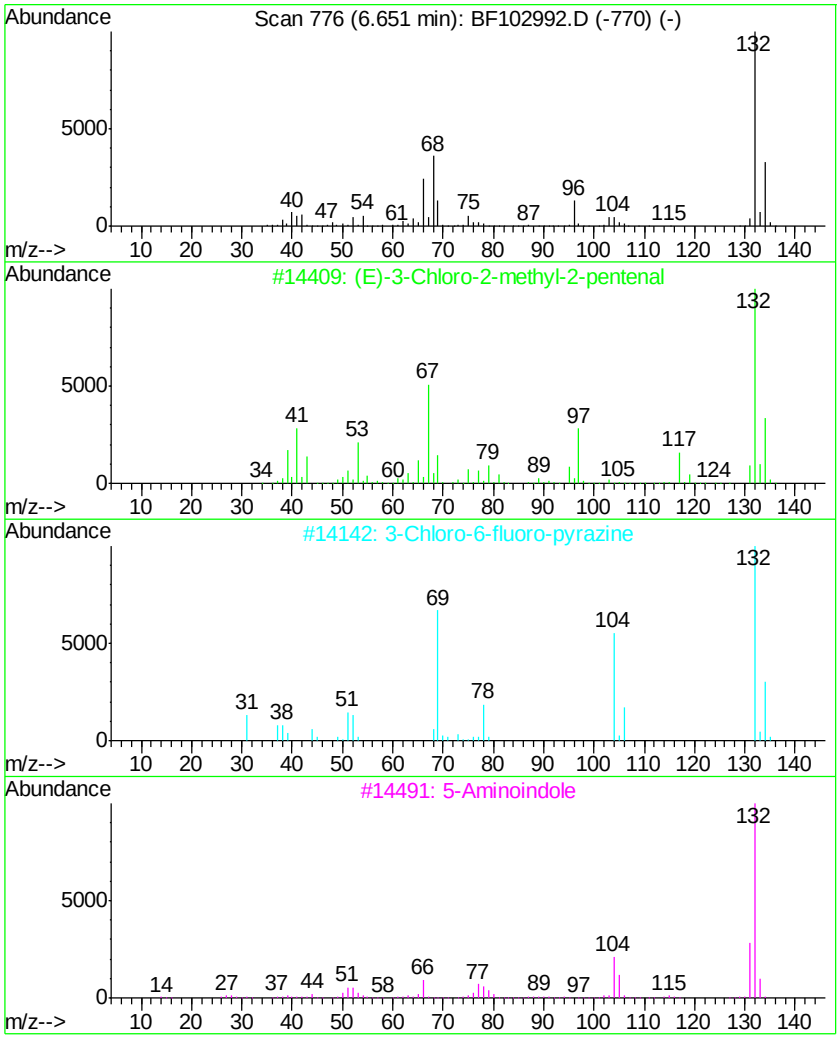
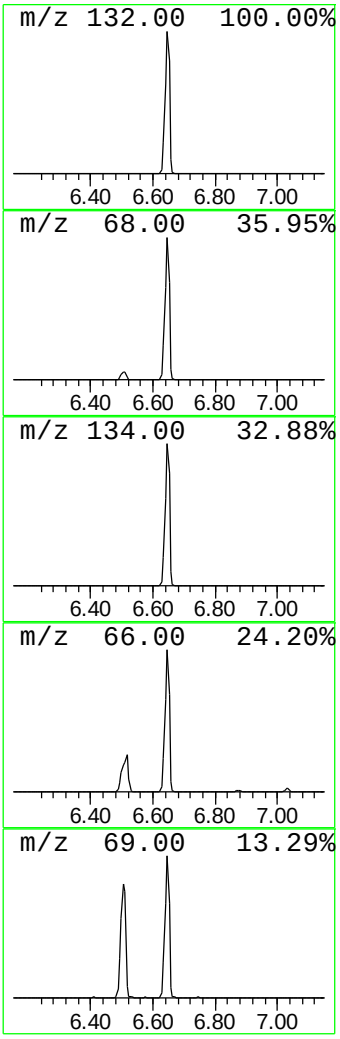
Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	69.73 ng	3650890	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : J1539-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MAIN-ST-LINE-3-EW@4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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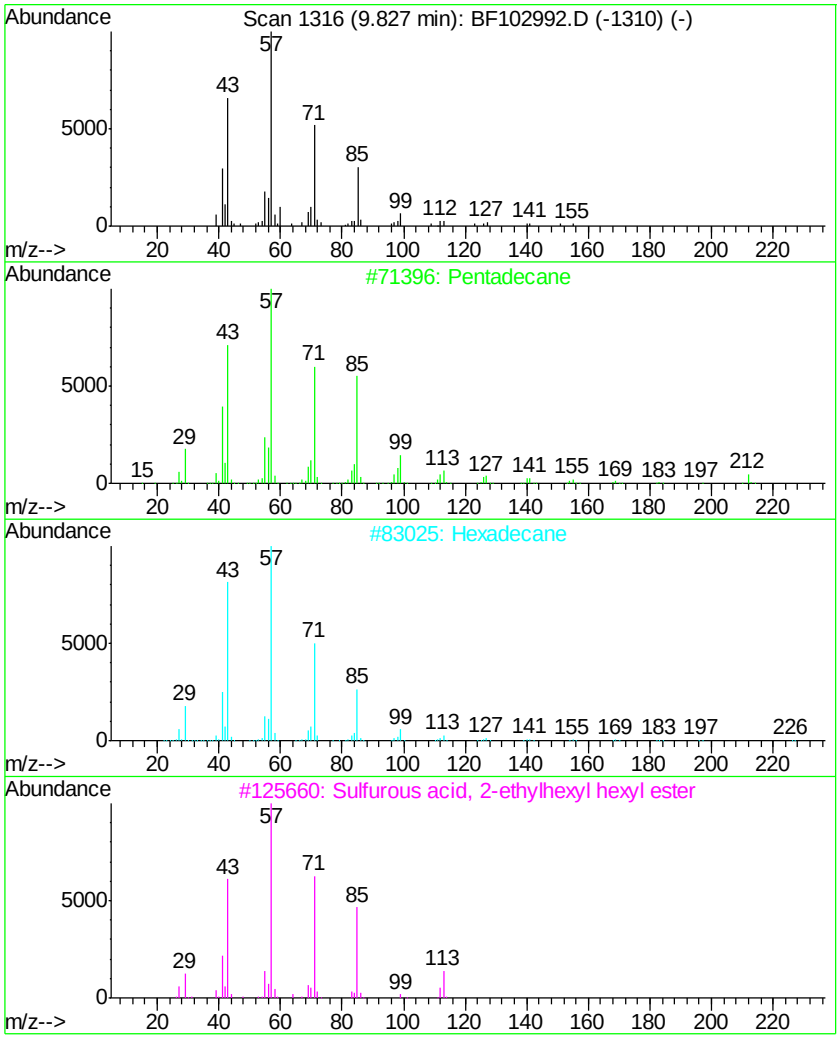
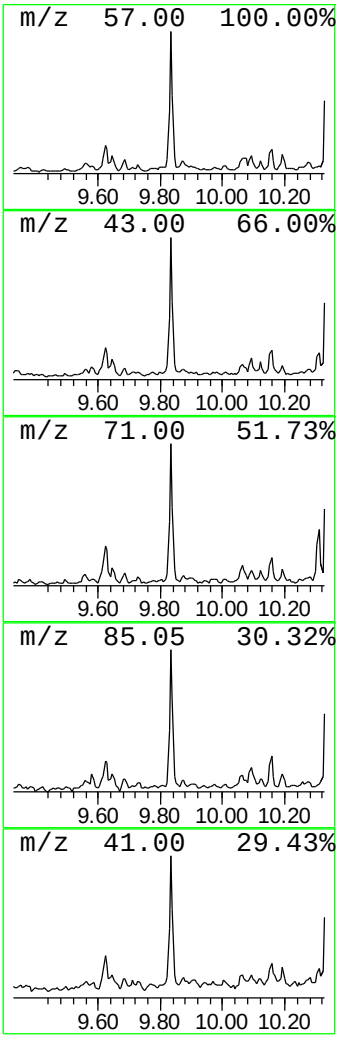
Peak Number 5 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	3.54 ng	213528	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Tridecane, 6-methyl-	198	C14H30	013287-21-3	72





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MAIN-ST-LINE-3-EW@4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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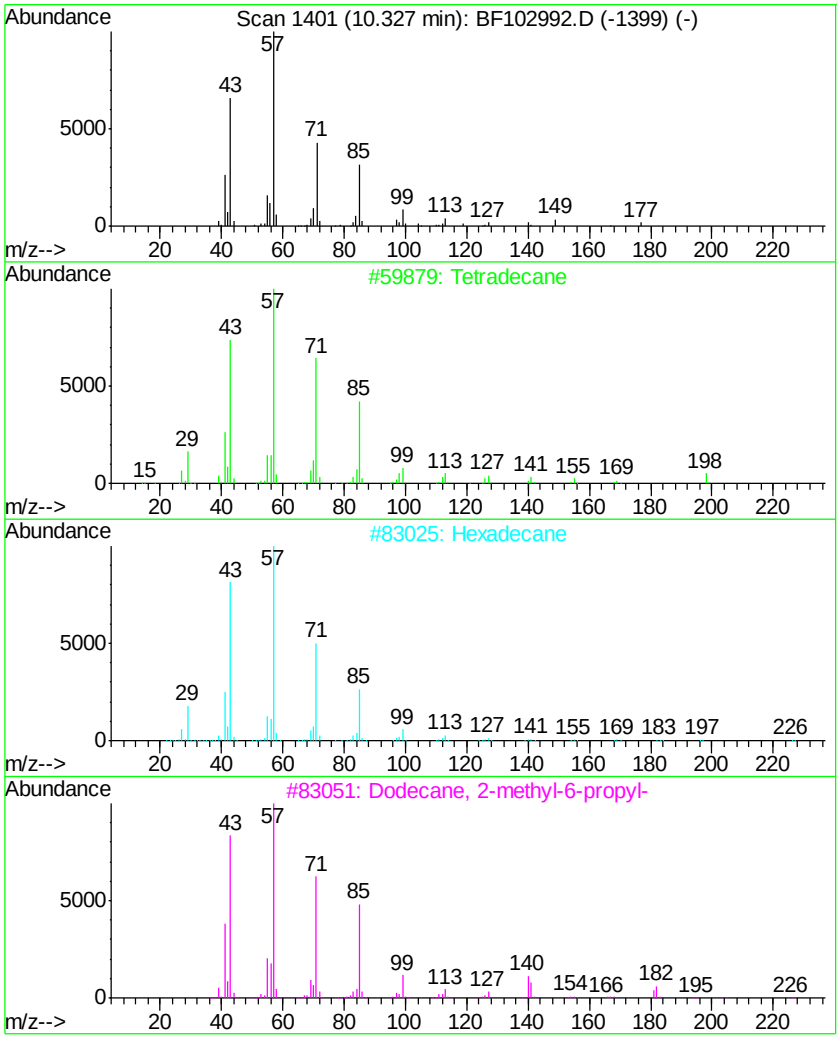
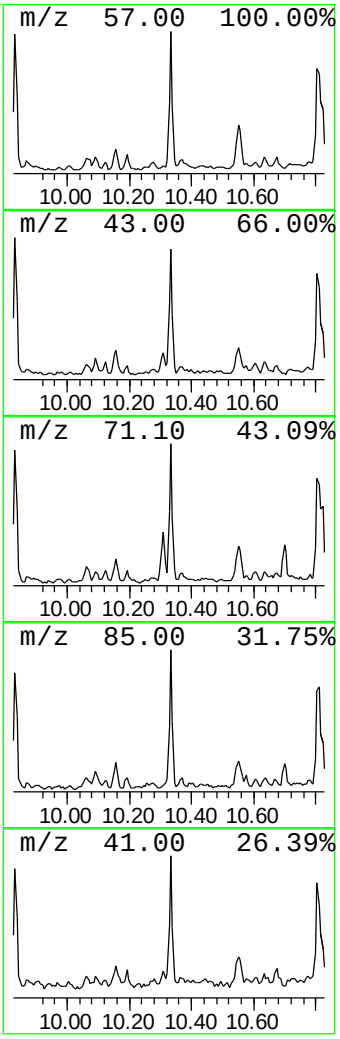
Peak Number 6 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	3.58 ng	215960	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Hexadecane	226	C16H34	000544-76-3	86
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72
4	Tridecane	184	C13H28	000629-50-5	72
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	64





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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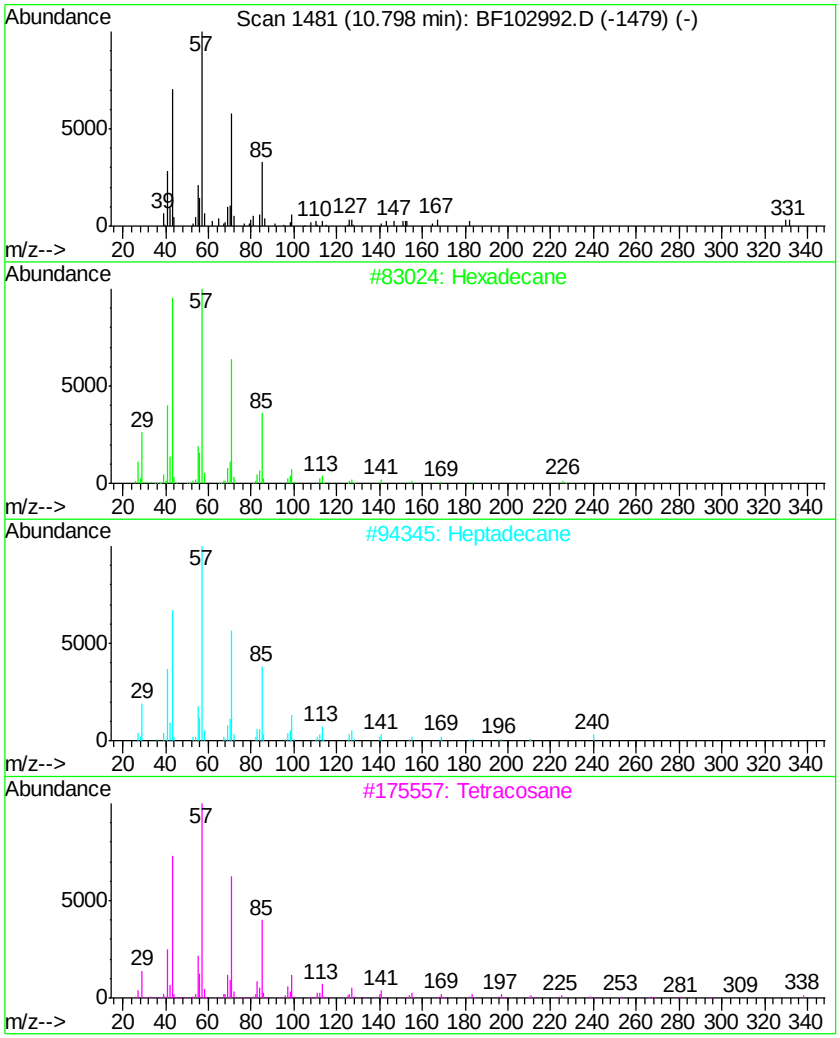
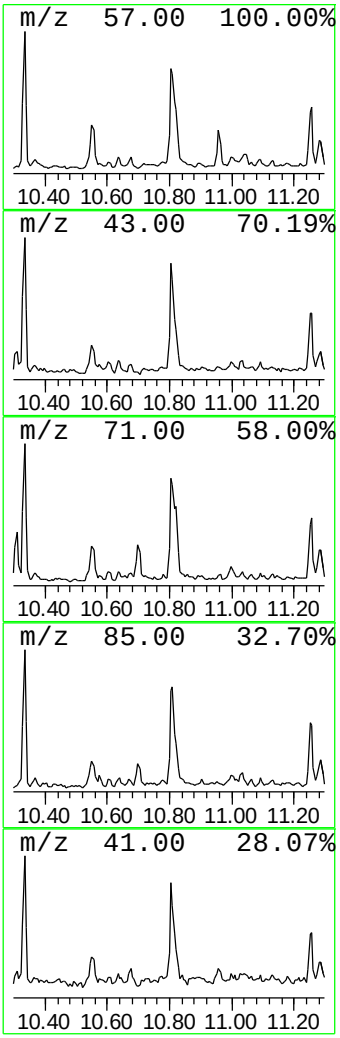
Peak Number 7 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	6.03 ng	290675	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Tetracosane	338	C24H50	000646-31-1	86
4	Tetratetracontane	619	C44H90	007098-22-8	83
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	80





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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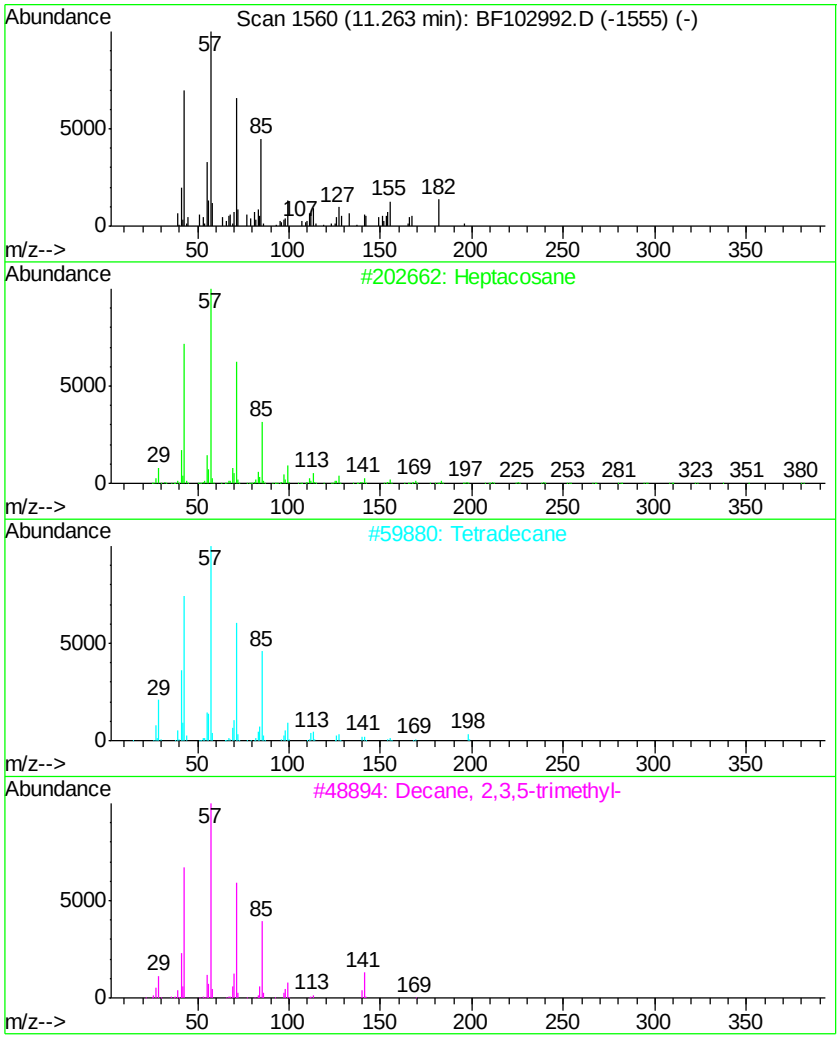
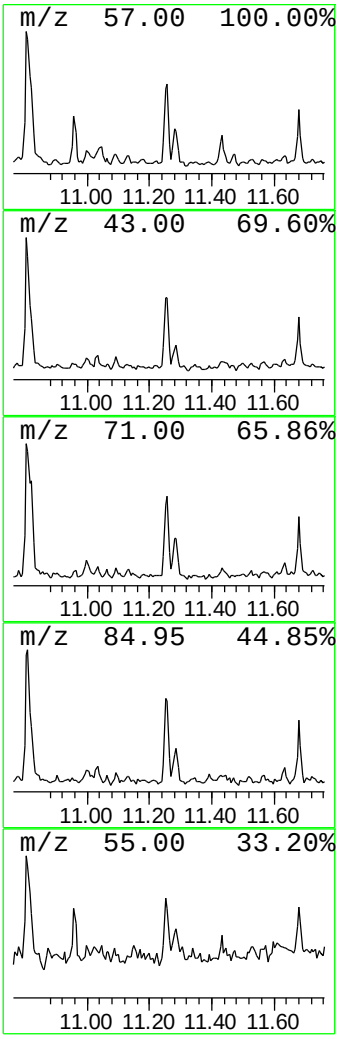
Peak Number 8 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	2.44 ng	117835	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
4	Tetracosane	338	C24H50	000646-31-1	86
5	Pentadecane	212	C15H32	000629-62-9	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102992.D
Acq On : 14 Feb 2018 16:30
Operator : SJ/JU
Sample : J1539-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MAIN-ST-LINE-3-EW@4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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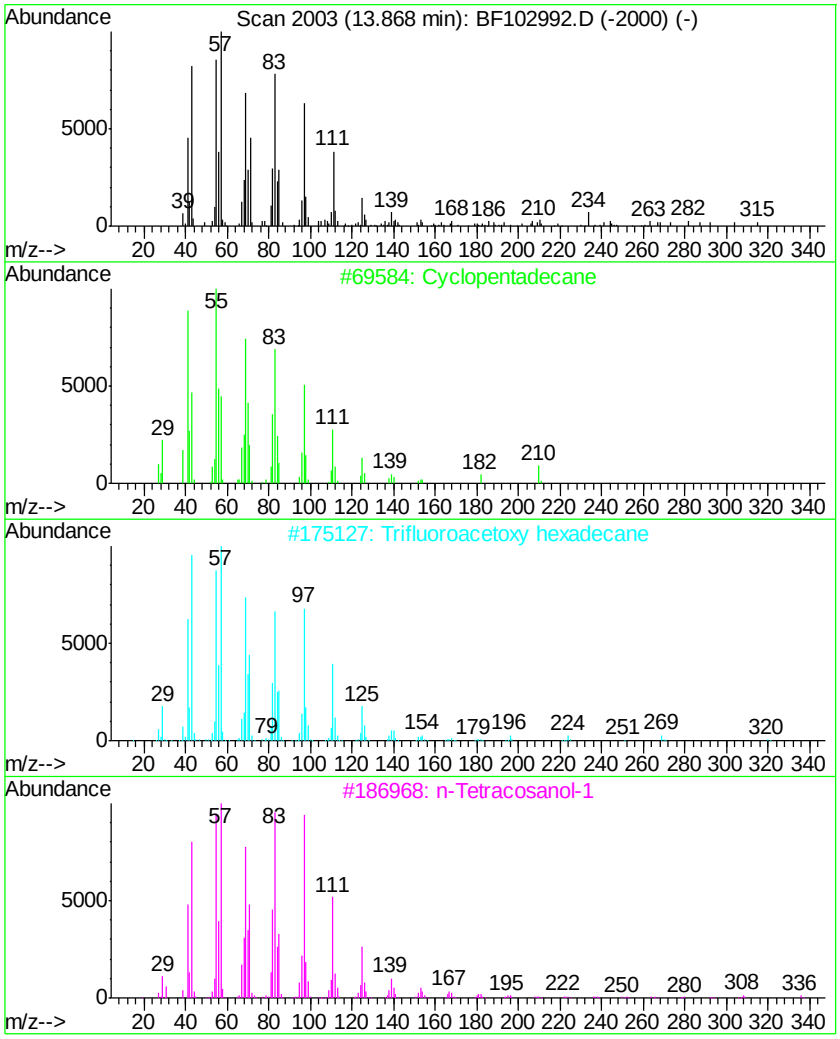
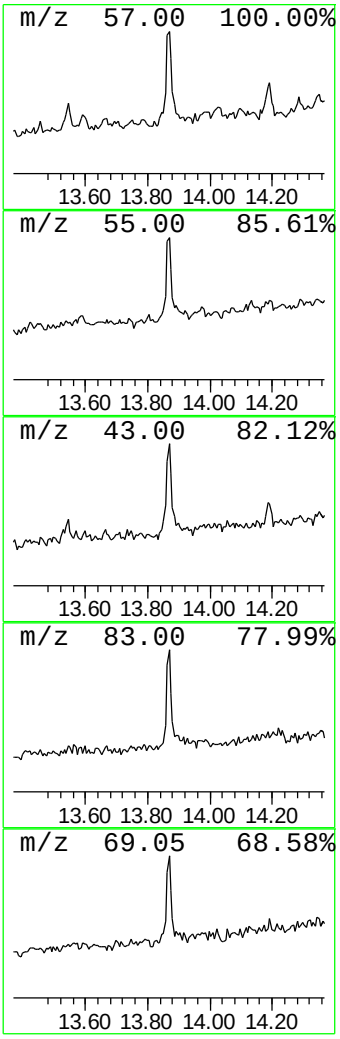
Peak Number 9 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.21 ng	214674	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	96
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102992.D
Acq On : 14 Feb 2018 16:30
Operator : SJ/JU
Sample : J1539-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MAIN-ST-LINE-3-EW@4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

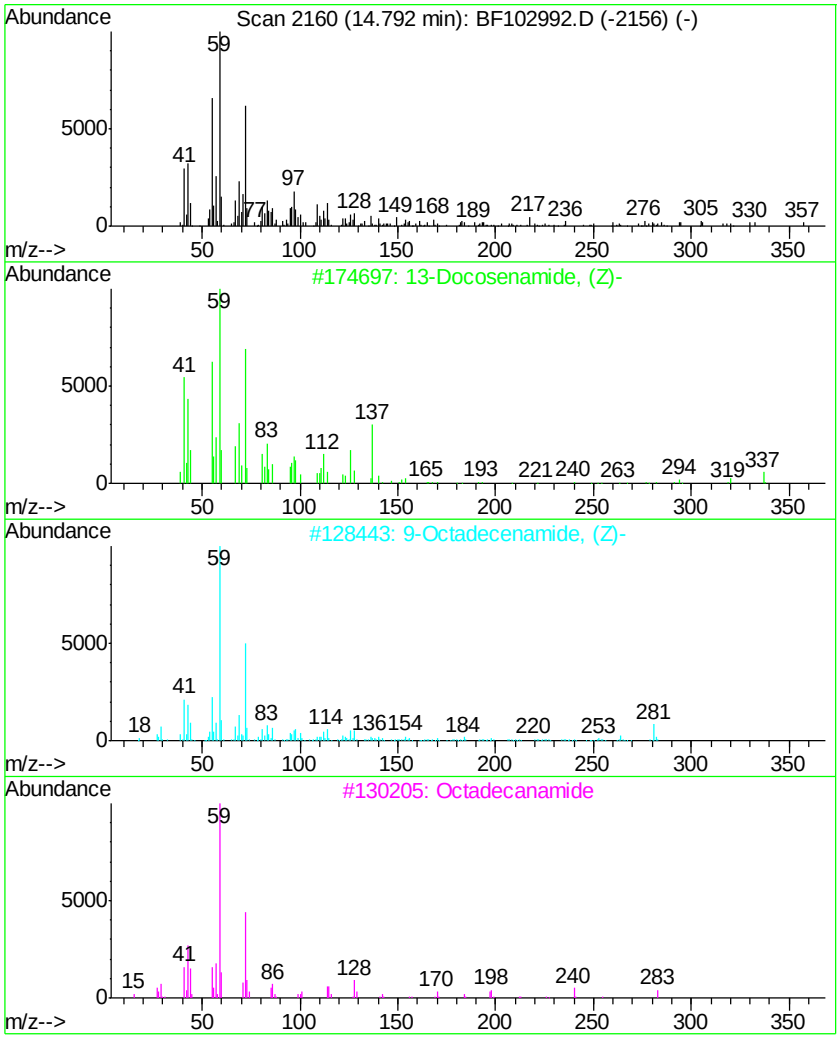
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

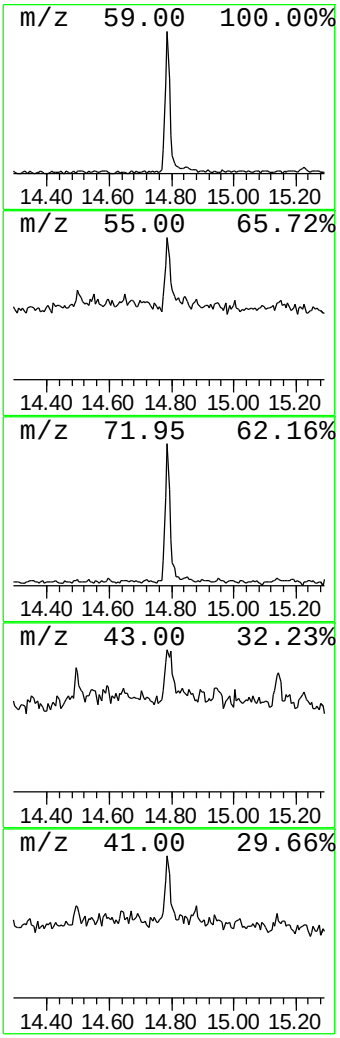
****

Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	5.30 ng	221313	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
3	Octadecanamide	283	C18H37NO	000124-26-5	72
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
5	Nonanamide	157	C9H19NO	001120-07-6	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021418\
Data File : BF102992.D
Acq On : 14 Feb 2018 16:30
Operator : SJ/JU
Sample : J1539-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MAIN-ST-LINE-3-EW@4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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...	2.15	19.0	ng	994577	1	6.87	1047130	20.0
2-Pentanone, 4-hy...	5.11	2.9	ng	149957	1	6.87	1047130	20.0
unknown6.65	6.65	69.7	ng	3650890	1	6.87	1047130	20.0
Pentadecane	9.83	3.5	ng	213528	3	9.91	1206500	20.0
Tetradecane	10.33	3.6	ng	215960	3	9.91	1206500	20.0
Hexadecane	10.80	6.0	ng	290675	4	11.40	964603	20.0
Heptacosane	11.26	2.4	ng	117835	4	11.40	964603	20.0
Cyclopentadecane	13.87	4.2	ng	214674	5	14.04	1019590	20.0
13-Docosenamide, ...	14.79	5.3	ng	221313	6	15.52	835295	20.0