LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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	2.140	4	9	16	rVB	237574	307443	6.82%	0.769%
2	5.110	511	514	522	rVB	111635	137824	3.06%	0.345%
3	5.504	576	581	584	rBV	4267697	4339886	96.29%	10.848%
4	6.516	747	753	772	rBV	4152906	4507091	100.00%	11.266%
5	6.657	772	777	780	rBV	4405296	4255180	94.41%	10.637%
6	6.886	812	816	819	rBV	1584360	1281200	28.43%	3.203%
7	7.039	838	842	846	rBV	2944153	2869228	63.66%	7.172%
8	7.451	906	912	915	rBV	2831616	2859104	63.44%	7.147%
9	8.169	1030	1034	1037	rBV	1980171	1618676	35.91%	4.046%
10	9.245	1212	1217	1220	rBV	3440923	3422034	75.93%	8.554%
11	9.316	1226	1229	1232	rVB	103150	75346	1.67%	0.188%
12	9.633	1279	1283	1286	rBV	412975	366227	8.13%	0.915%
13	9.845	1311	1319	1324	rBV	247134	228951	5.08%	0.572%
14	9.927	1329	1333	1341	rVB	1520826	1511112	33.53%	3.777%
15	10.169	1371	1374	1378	rBV2	46198	52064	1.16%	0.130%
16	10.322	1397	1400	1402	rBV	63096	56280	1.25%	0.141%
17	10.345	1402	1404	1407	rVB	244741	185831	4.12%	0.465%
18	10.569	1437	1442	1444	rBV	58505	74205	1.65%	0.185%
19	10.716	1463	1467	1475	rVB	1818531	1816122	40.29%	4.540%
20	10.821	1482	1485	1490	rVB	173071	182411	4.05%	0.456%
21	11.269	1558	1561	1563	rBV	119541	92530	2.05%	0.231%
22	11.298	1563	1566	1572	rVB2	39334	45543	1.01%	0.114%
23	11.410	1582	1585	1589	rBV	1174383	1143980	25.38%	2.860%
24	11.692	1630	1633	1637	rBV	61771	54435	1.21%	0.136%
25	11.927	1670	1673	1682	rBV2	87537	102129	2.27%	0.255%
26	12.998	1851	1855	1858	rBV	2334322	2092366	46.42%	5.230%
27	13.474	1924	1936	1938	rBV3	337930	928520	20.60%	2.321%
28	13.774	1968	1987	1999	rBV3	575183	2656818	58.95%	6.641%
29	13.880	2002	2005	2018	rVB	539737	588298	13.05%	1.471%
30	14.051	2031	2034	2038	rBV	996462	1000270	22.19%	2.500%
31	14.515	2110	2113	2116	rBV	99828	107958	2.40%	0.270%
32	15.162	2221	2223	2226	rVB	66263	55374	1.23%	0.138%
33	15.539	2283	2287	2294	rVB	642252	860903	19.10%	2.152%
34	15.998	2362	2365	2370	rVB	94744	129158	2.87%	0.323%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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

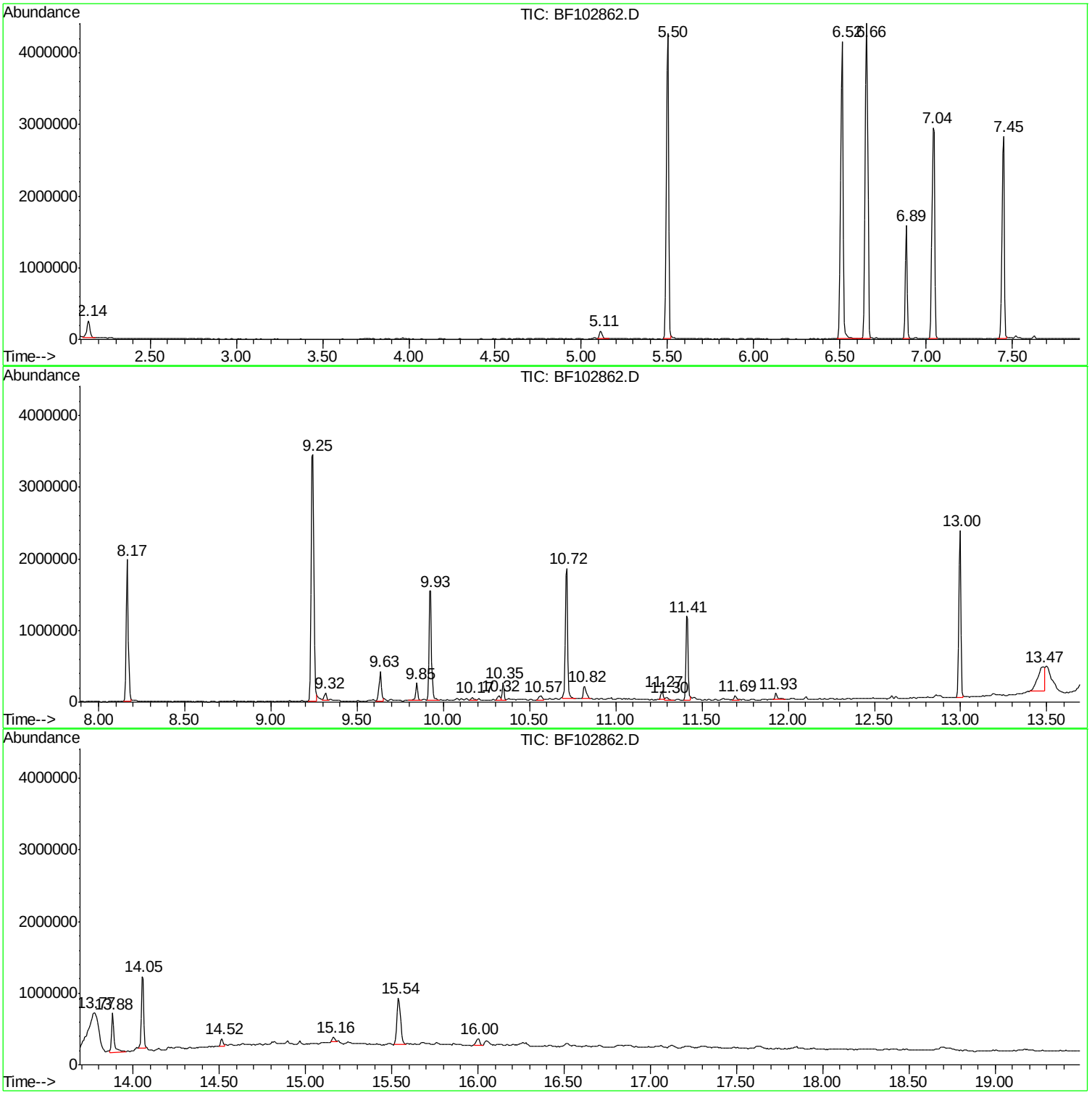
Sum of corrected areas: 40004497

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-9

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\BF020818\
Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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

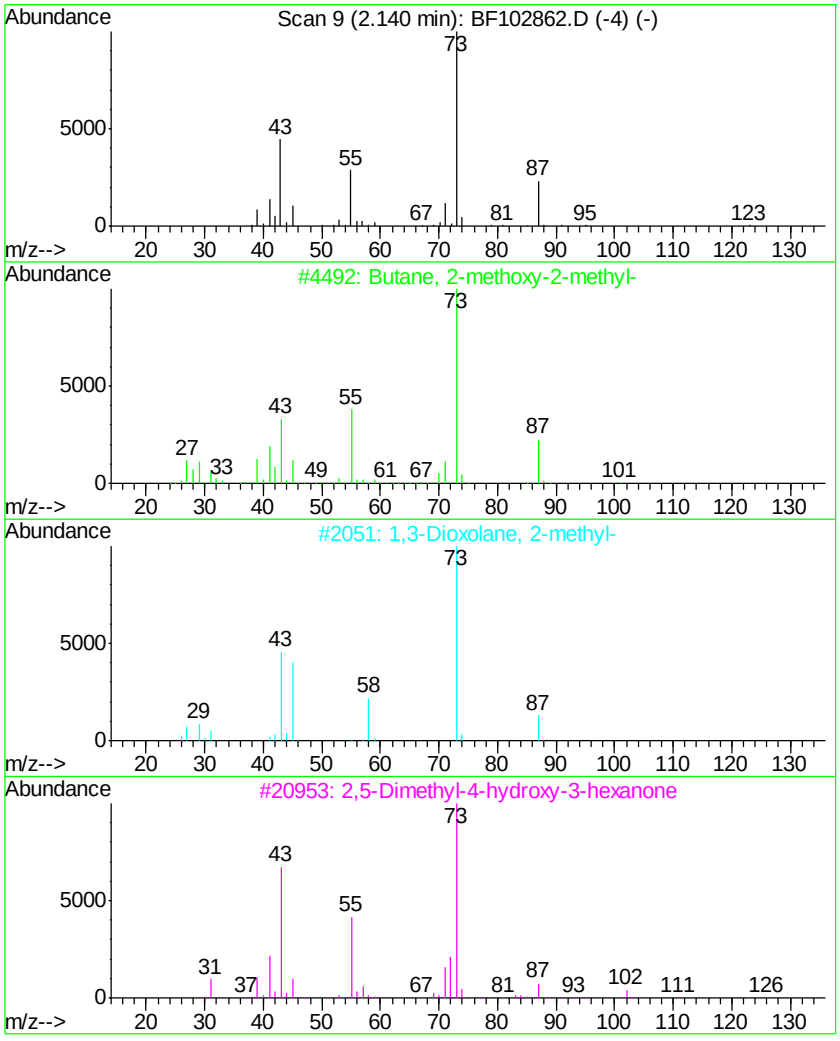
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

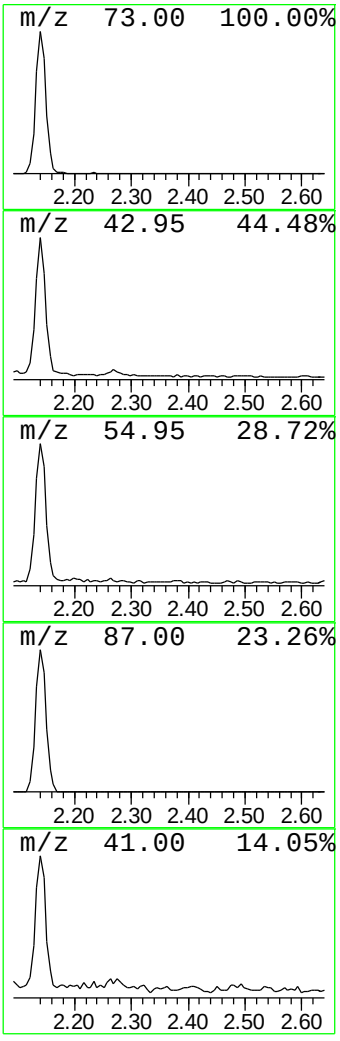
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	4.80 ng	307443	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3	2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	28
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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

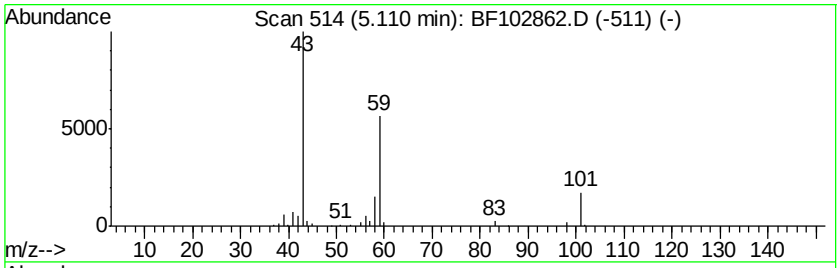
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

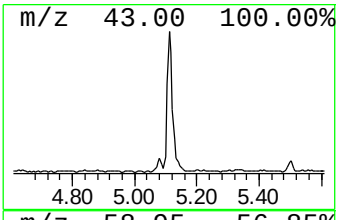
****

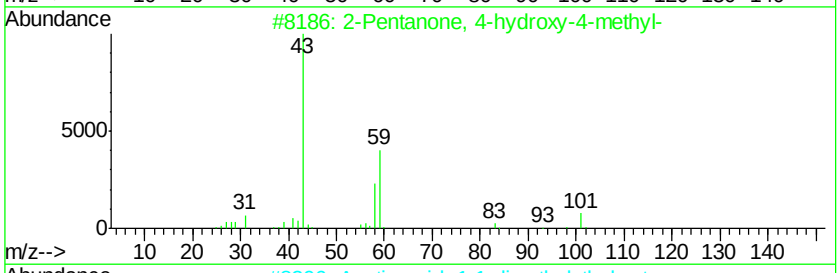
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

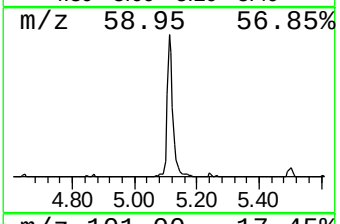
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	2.15 ng	137824	1,4-Dichlorobenzene-d4	6.89

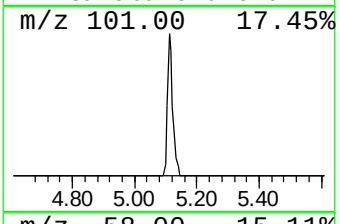
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27

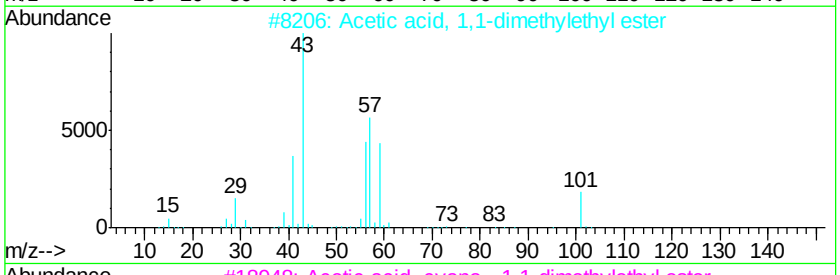


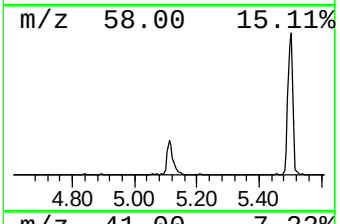


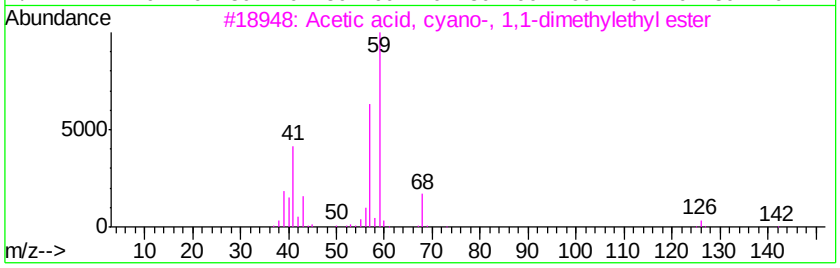


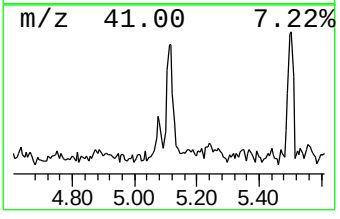












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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

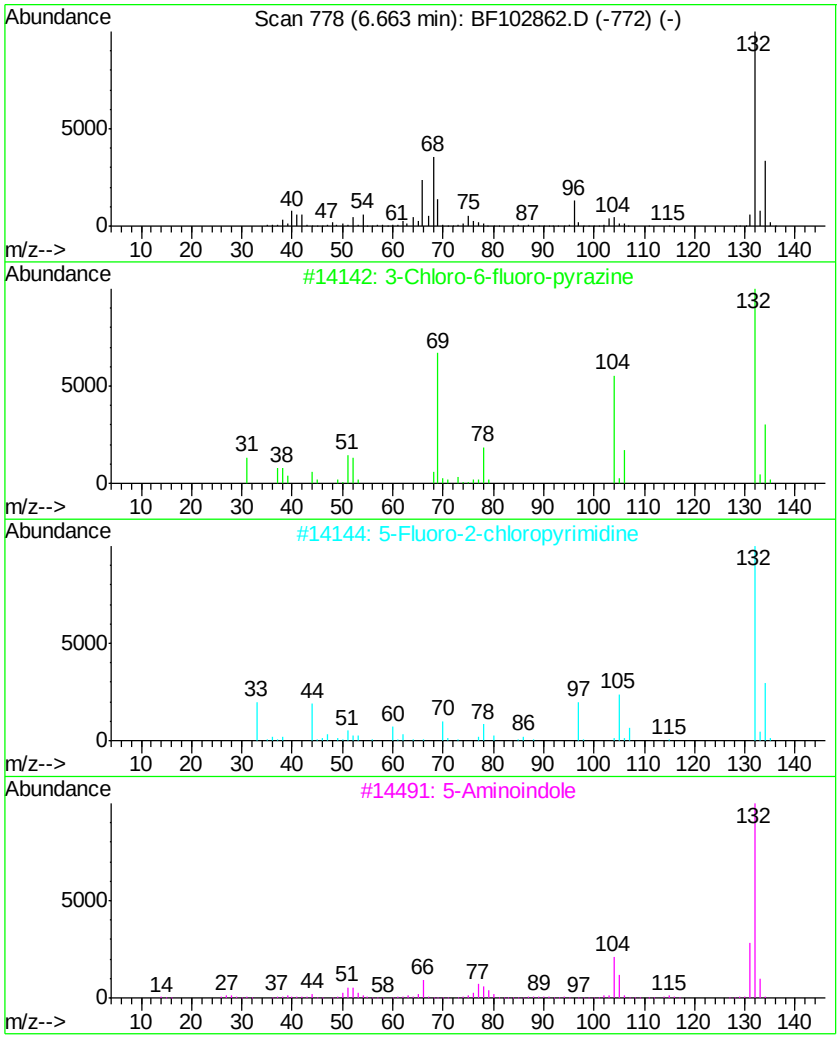
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

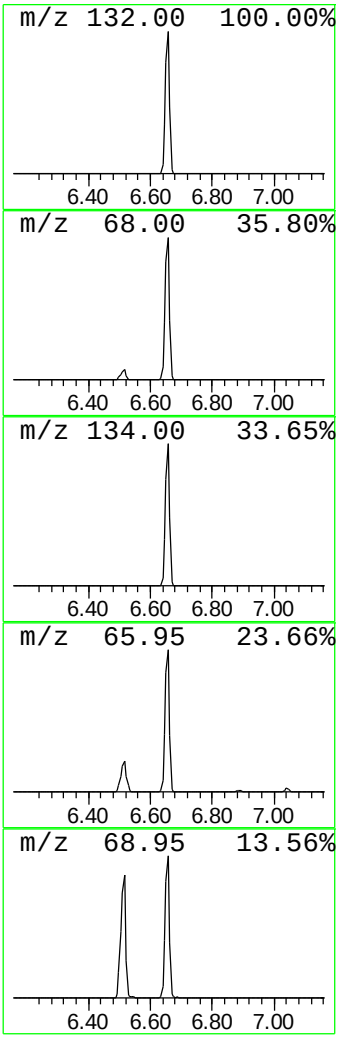
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	66.42 ng	4255180	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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

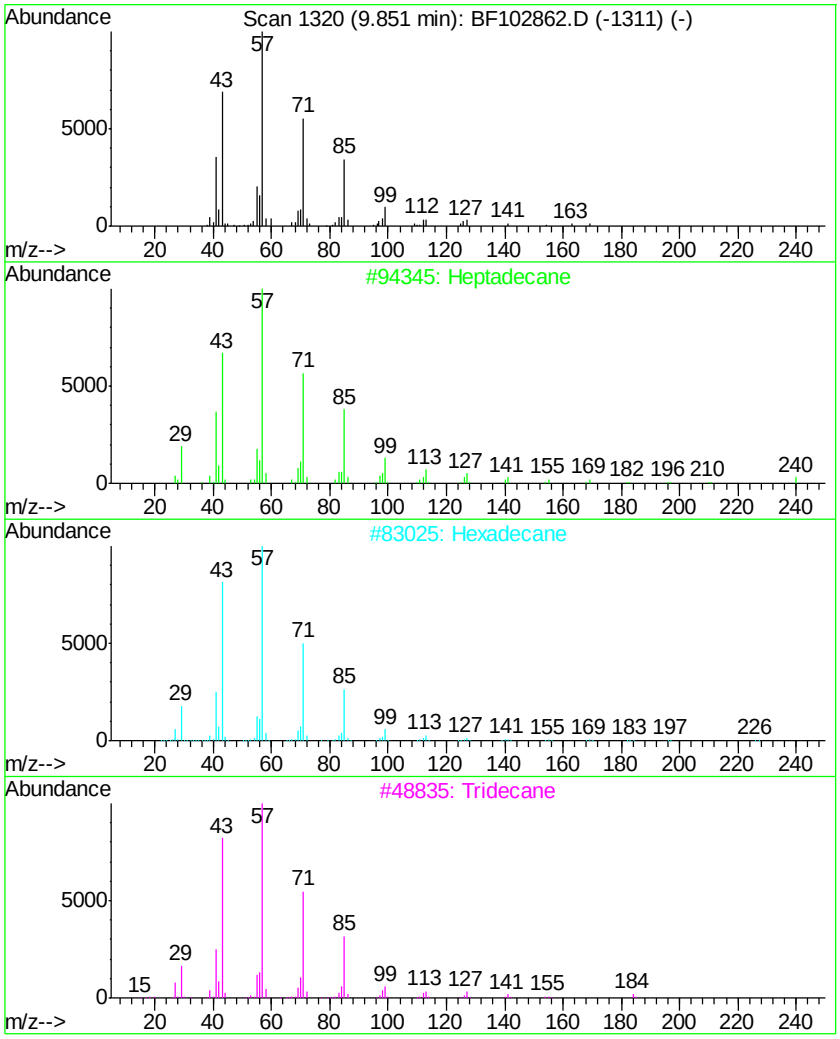
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

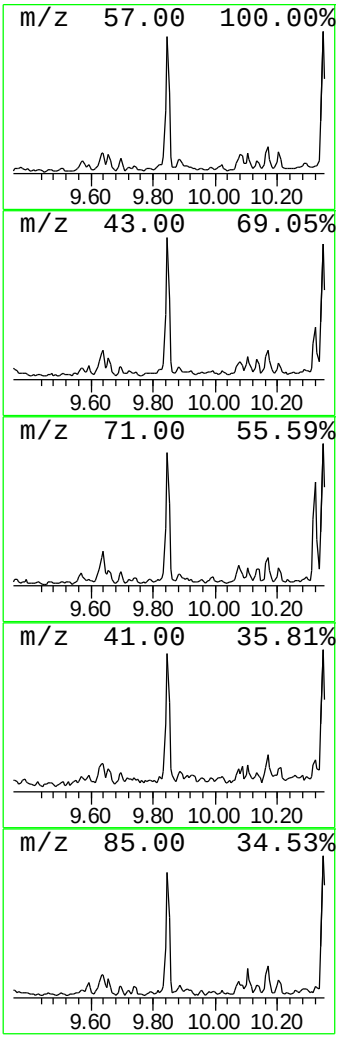
****

Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	3.03 ng	228951	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Tetradecane	198	C14H30	000629-59-4	90
5	Tridecane, 4,8-dimethyl-	212	C15H32	055030-62-1	86





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Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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

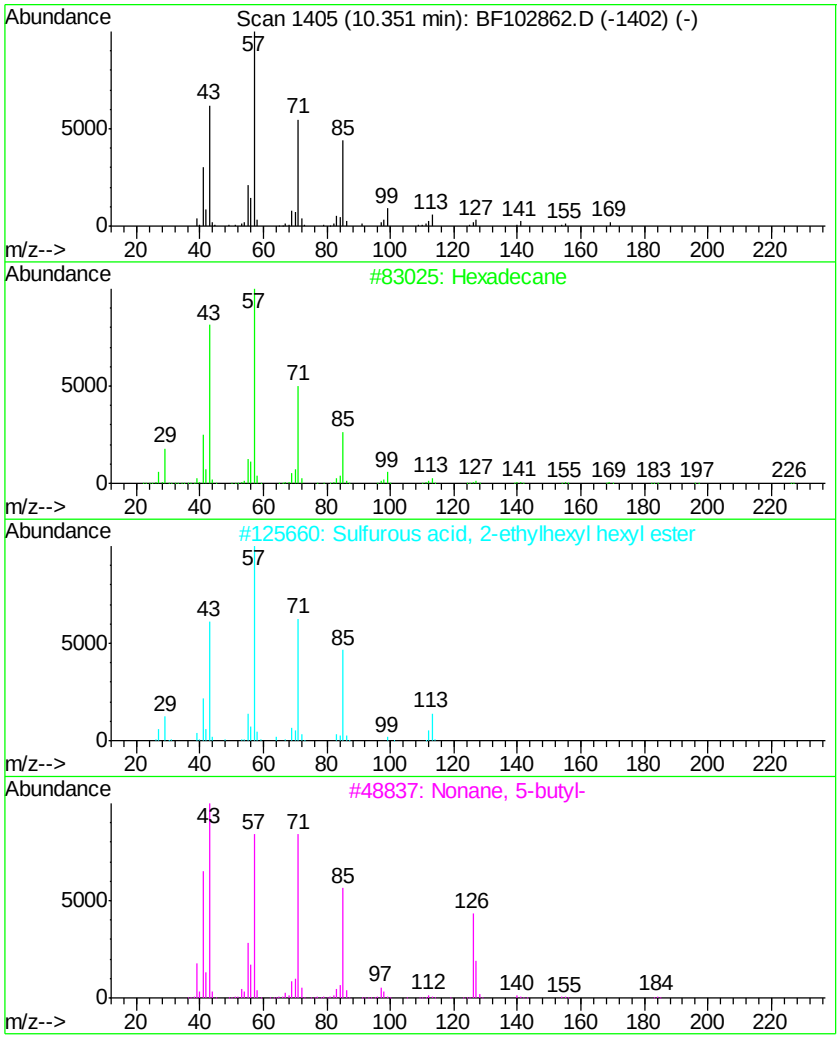
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

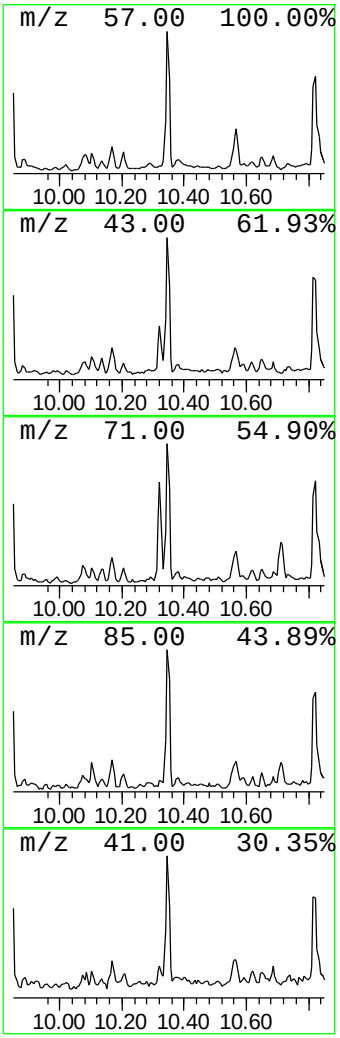
****

Peak Number 6 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.46 ng	185831	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	86
3	Nonane, 5-butyl-	184	C13H28	017312-63-9	72
4	Tridecane	184	C13H28	000629-50-5	59
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-9

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

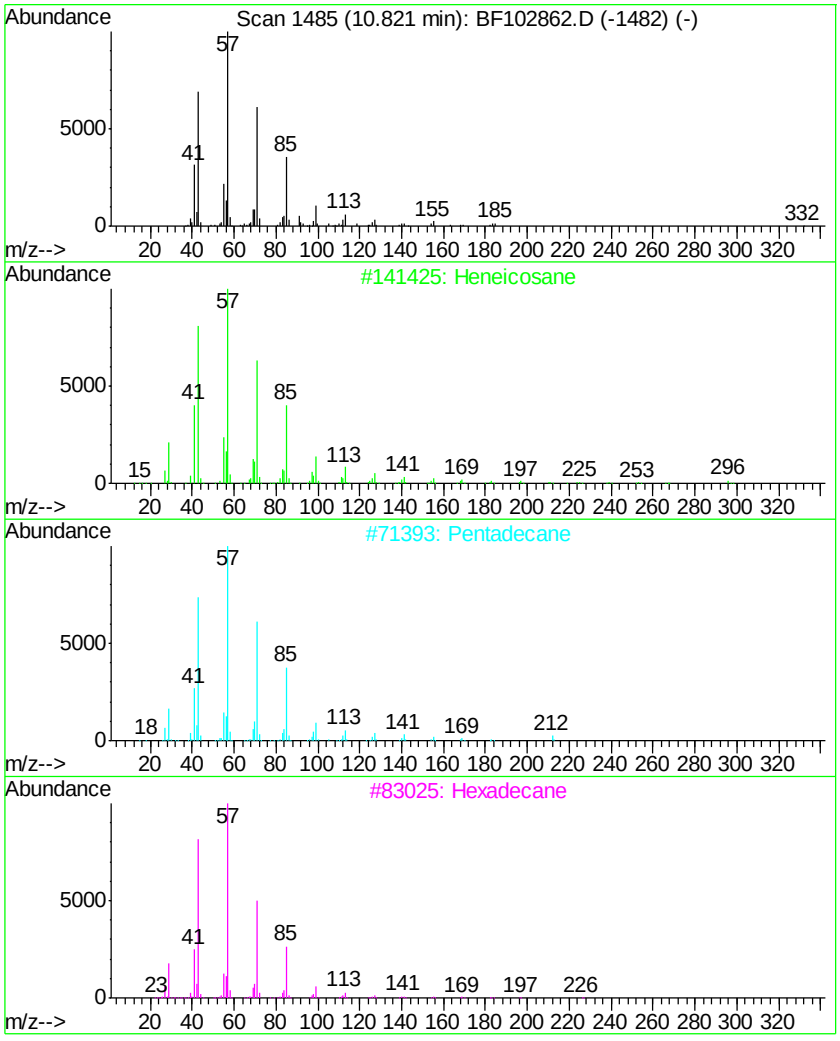
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

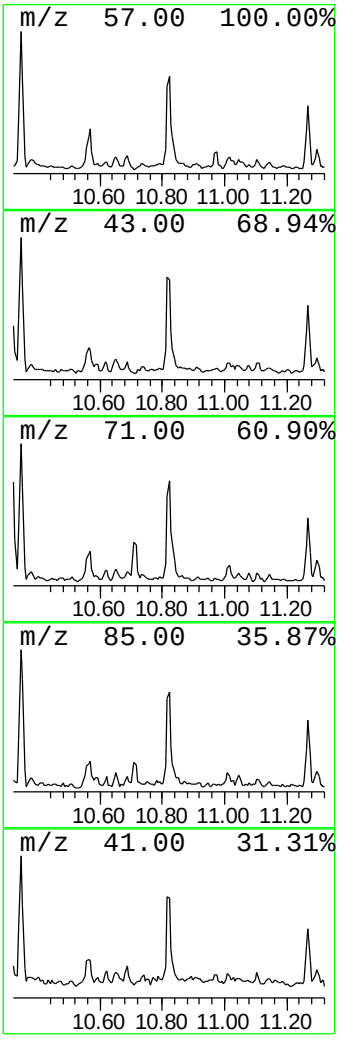
****

Peak Number 7 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.19 ng	182411	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Eicosane	282	C20H42	000112-95-8	87
5	Octadecane	254	C18H38	000593-45-3	86





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Acq On : 8 Feb 2018 18:01
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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

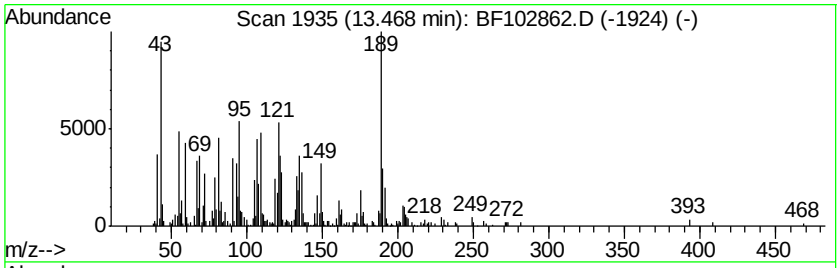
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

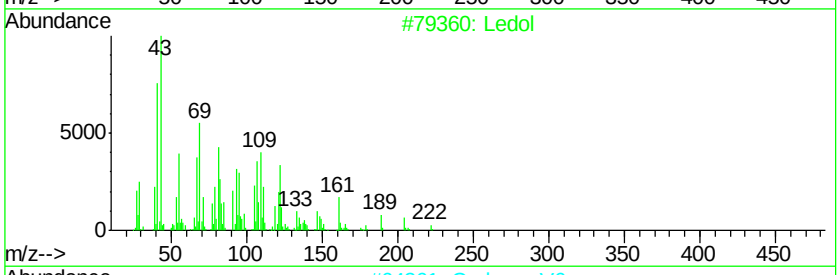
****

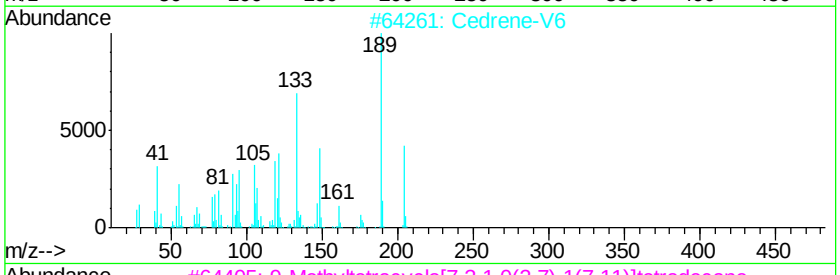
Peak Number 8 unknown13.47 Concentration Rank 4

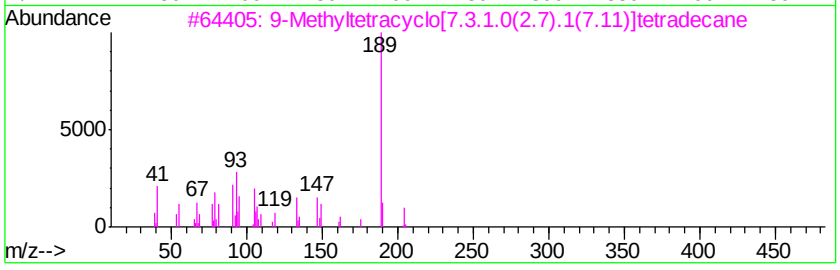
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	18.57 ng	928520	Chrysene-d12	14.06

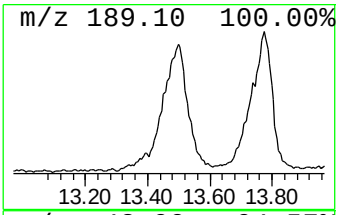
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ledol	222	C15H26O	000577-27-5	48
2	Cedrene-V6	204	C15H24	1000162-76-8	35
3	9-Methyltetracyclo[7.3.1.0(2.7)....	204	C15H24	1000215-30-5	30
4	Propenone, 1-(4-fluorophenyl)-3-...	312	C17H13FN2OS	1000263-71-8	25
5	Caryophyllene oxide	220	C15H24O	001139-30-6	22

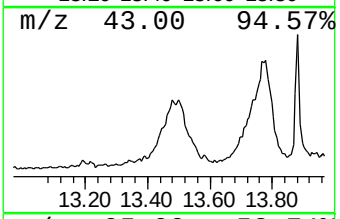


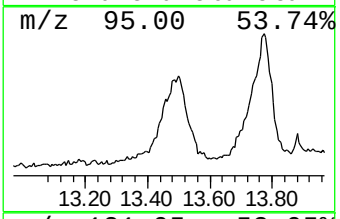


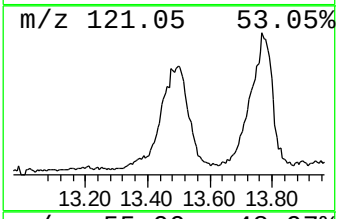


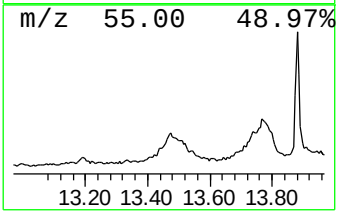












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Data File : BF102862.D
Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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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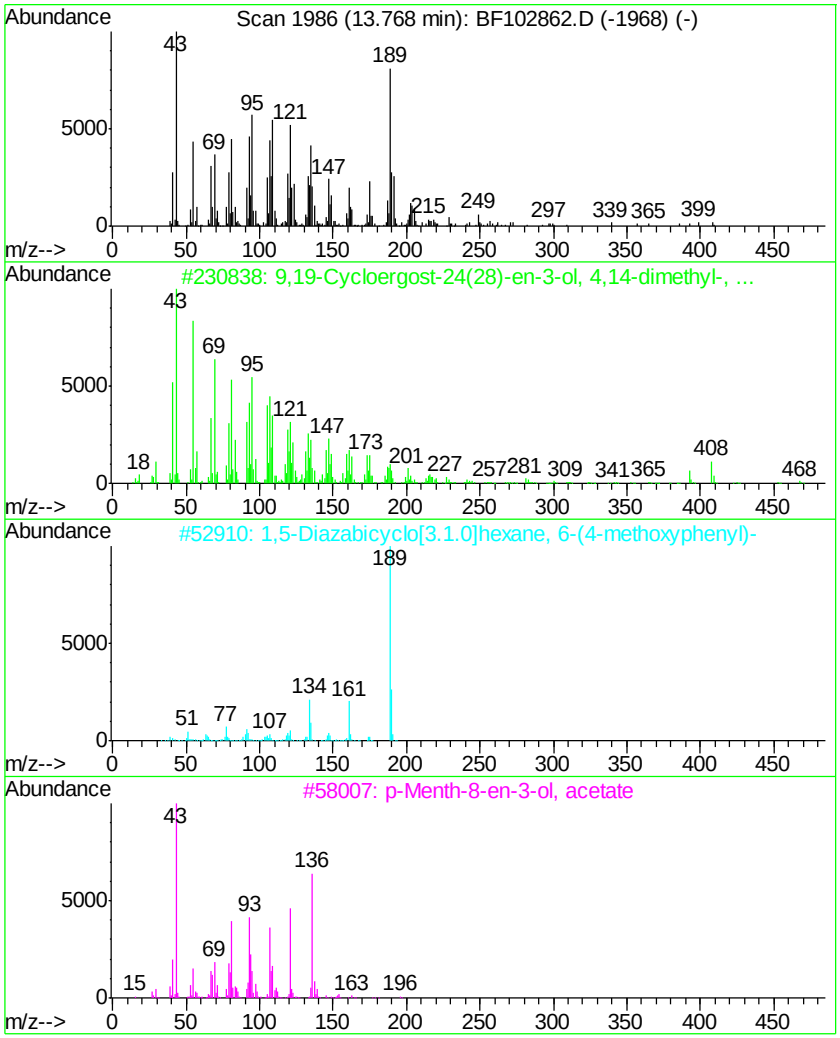
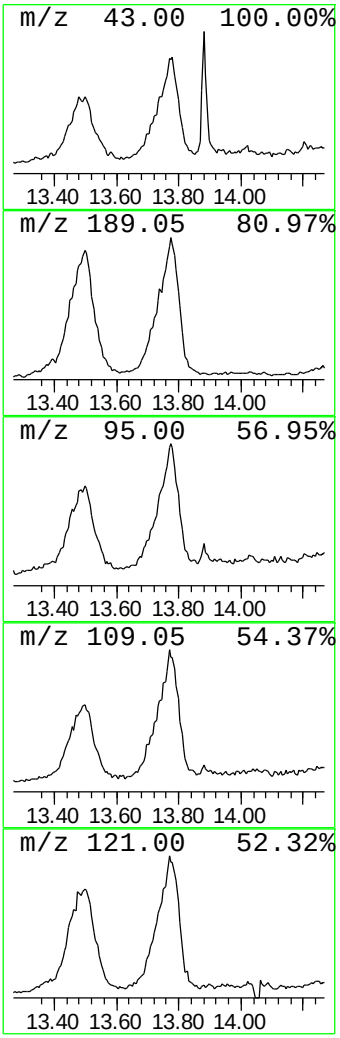
Peak Number 9 9,19-Cycloergost-24(28)-en-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	53.12 ng	2656820	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,19-Cycloergost-24(28)-en-3-ol,...	468	C32H52O2	010376-42-8	53
2	1,5-Diazabicyclo[3.1.0]hexane, 6...	190	C11H14N2O	1000337-54-5	18
3	p-Menth-8-en-3-ol, acetate	196	C12H20O2	000089-49-6	15
4	Acetic acid, 1,7,7-trimethyl-bic...	196	C12H20O2	092618-89-8	15
5	3H-1,3,4-Benzotriazepin-2-one, 1...	189	C10H11N3O	105999-05-1	14





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Instrument : BNA_F
ClientSampleId : 3N-9

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

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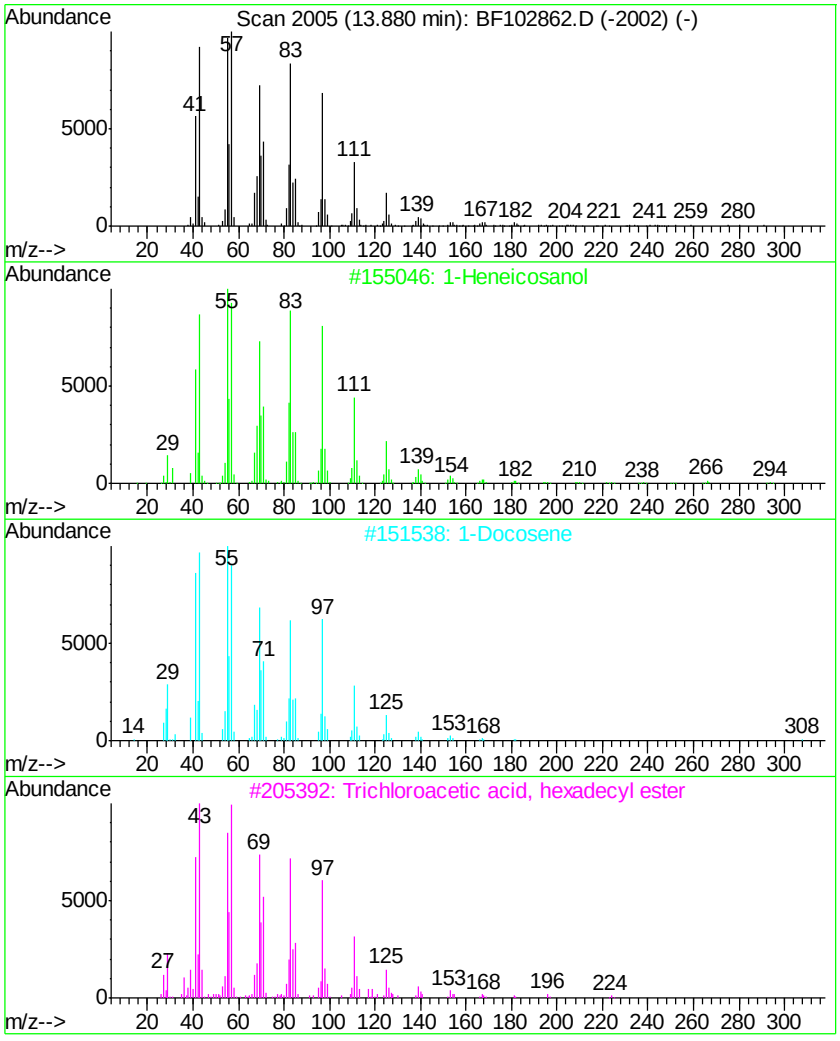
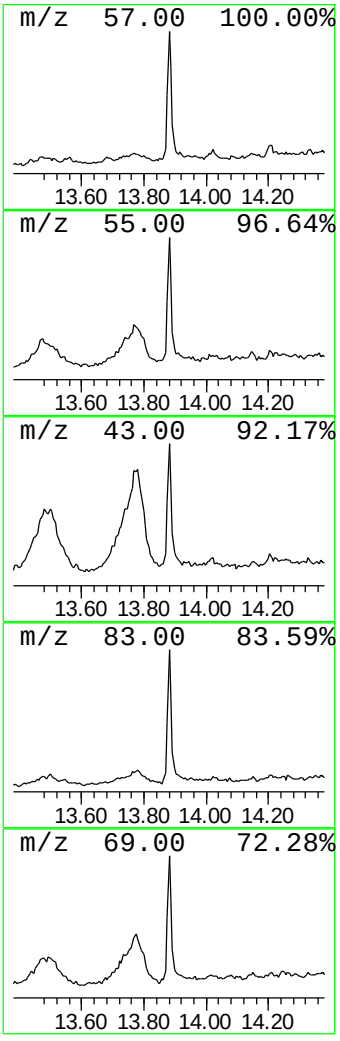
Peak Number 10 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	11.76 ng	588298	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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Operator : SJ/JU
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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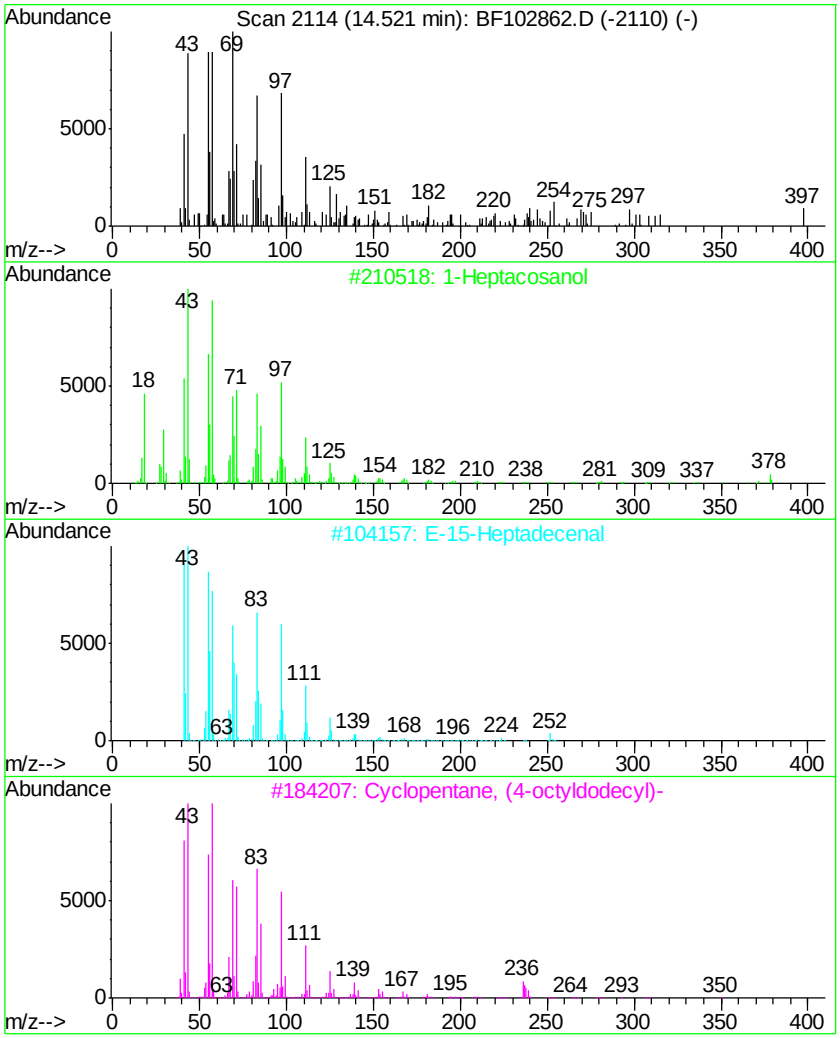
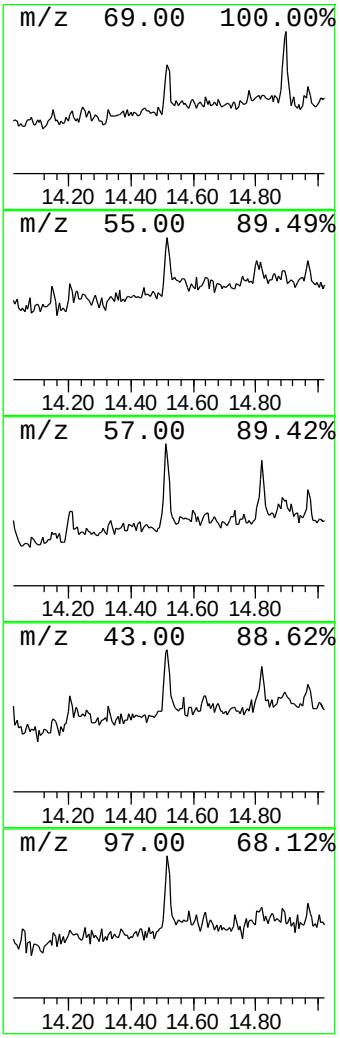
Peak Number 11 1-Heptacosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.16 ng	107958	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	87
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	83
3	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	76
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	74
5	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	74





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Operator : SJ/JU
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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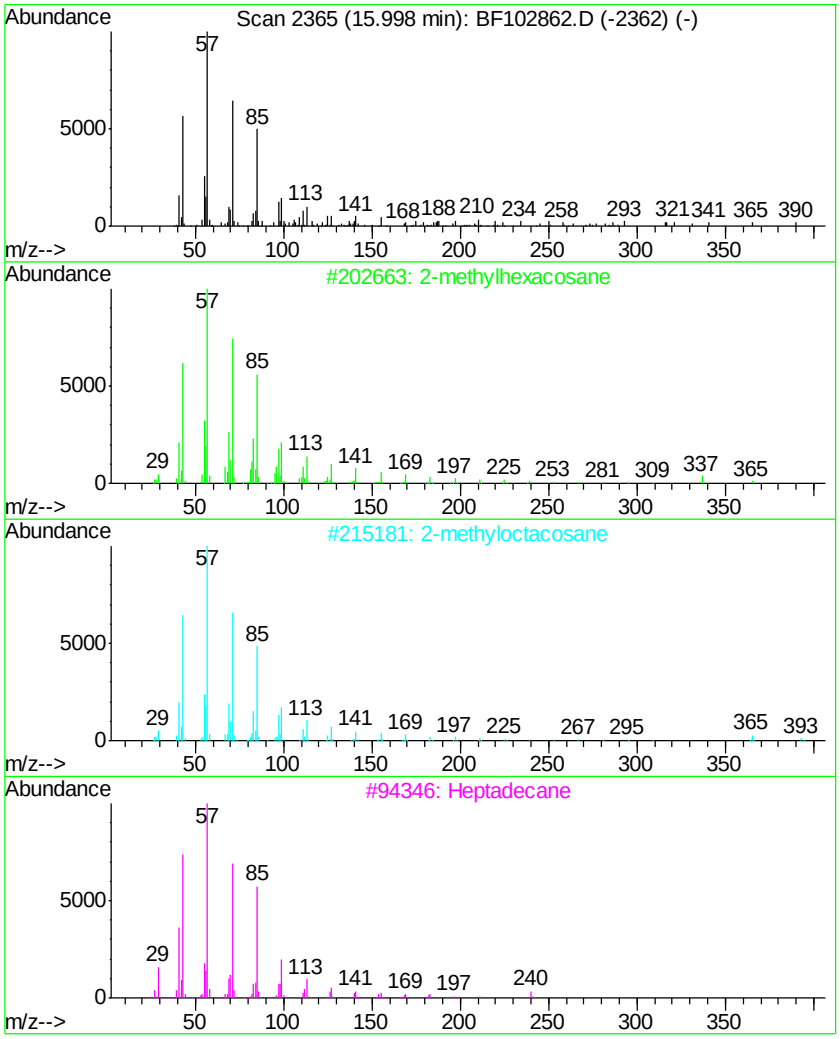
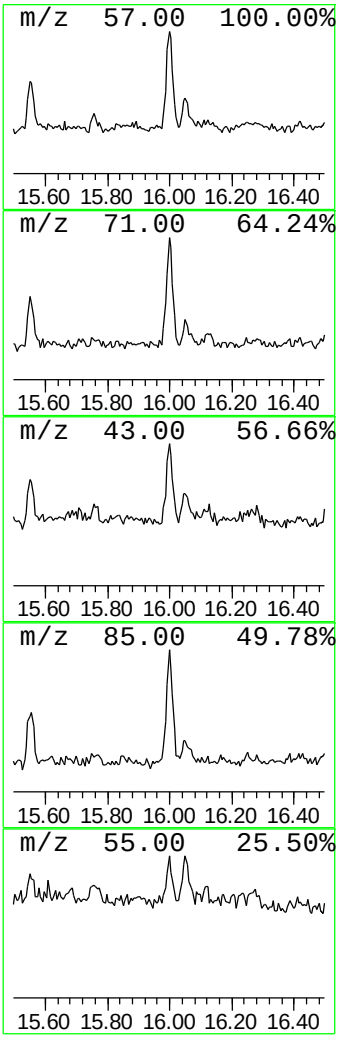
Peak Number 12 2-methylhexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	3.00 ng	129158	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methylhexacosane	380	C27H56	1000376-72-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Heptadecane	240	C17H36	000629-78-7	86
4	Hexatriacontane	507	C36H74	000630-06-8	86
5	Heptacosane	380	C27H56	000593-49-7	86





Tentatively Identified Compound (LSC) summary

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Acq On : 8 Feb 2018 18:01
Operator : SJ/JU
Sample : J1470-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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...	2.14	4.8	ng	307443	1	6.89	1281200	20.0
2-Pentanone, 4-hy...	5.11	2.1	ng	137824	1	6.89	1281200	20.0
unknown6.66	6.66	66.4	ng	4255180	1	6.89	1281200	20.0
Heptadecane	9.85	3.0	ng	228951	3	9.92	1511110	20.0
Hexadecane	10.35	2.5	ng	185831	3	9.92	1511110	20.0
Heneicosane	10.82	3.2	ng	182411	4	11.42	1143980	20.0
unknown13.47	13.47	18.6	ng	928520	5	14.06	1000270	20.0
9,19-Cycloergost-...	13.77	53.1	ng	2656820	5	14.06	1000270	20.0
1-Heneicosanol	13.88	11.8	ng	588298	5	14.06	1000270	20.0
1-Heptacosanol	14.52	2.2	ng	107958	5	14.06	1000270	20.0
2-methylhexacosane	16.00	3.0	ng	129158	6	15.54	860903	20.0