LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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	2.163	6	13	21	rBV	672823	884159	5.91%	1.634%
2	3.628	257	262	272	rBV	341556	537669	3.60%	0.994%
3	4.528	404	415	418	rBV	6285403	14954221	100.00%	27.644%
4	5.140	509	519	522	rVB	4587408	9900443	66.21%	18.302%
5	6.504	747	751	765	rBV	1481062	1370585	9.17%	2.534%
6	6.651	772	776	779	rBV	321708	261357	1.75%	0.483%
7	6.887	812	816	819	rBV	1290012	1139569	7.62%	2.107%
8	7.040	838	842	846	rBV	3302257	3189444	21.33%	5.896%
9	7.204	867	870	877	rVB	519482	396352	2.65%	0.733%
10	7.445	906	911	915	rBV	2534284	2616574	17.50%	4.837%
11	8.169	1030	1034	1037	rBV	1698696	1439432	9.63%	2.661%
12	9.245	1212	1217	1220	rBV	4170585	3944197	26.38%	7.291%
13	9.316	1226	1229	1232	rBV2	228939	248668	1.66%	0.460%
14	9.633	1280	1283	1286	rBV2	1040205	1084738	7.25%	2.005%
15	9.792	1306	1310	1312	rBV	545536	605741	4.05%	1.120%
16	9.833	1312	1317	1321	rVV2	973458	1152868	7.71%	2.131%
17	9.928	1330	1333	1336	rVB	1331862	1262444	8.44%	2.334%
18	9.957	1336	1338	1340	rBV2	318017	345800	2.31%	0.639%
19	10.175	1372	1375	1378	rBV2	502853	653355	4.37%	1.208%
20	10.239	1384	1386	1388	rBV3	330552	357508	2.39%	0.661%
21	10.333	1399	1402	1407	rBV2	1199114	1618069	10.82%	2.991%
22	10.845	1485	1489	1492	rBV	1610167	2127070	14.22%	3.932%
23	13.016	1855	1858	1865	rVB	1268716	1411115	9.44%	2.609%
24	13.886	2003	2006	2013	rVB	645917	772018	5.16%	1.427%
25	14.063	2033	2036	2042	rVB	951152	904190	6.05%	1.671%
26	15.545	2283	2288	2295	rVB	683078	918257	6.14%	1.697%

Sum of corrected areas: 54095843

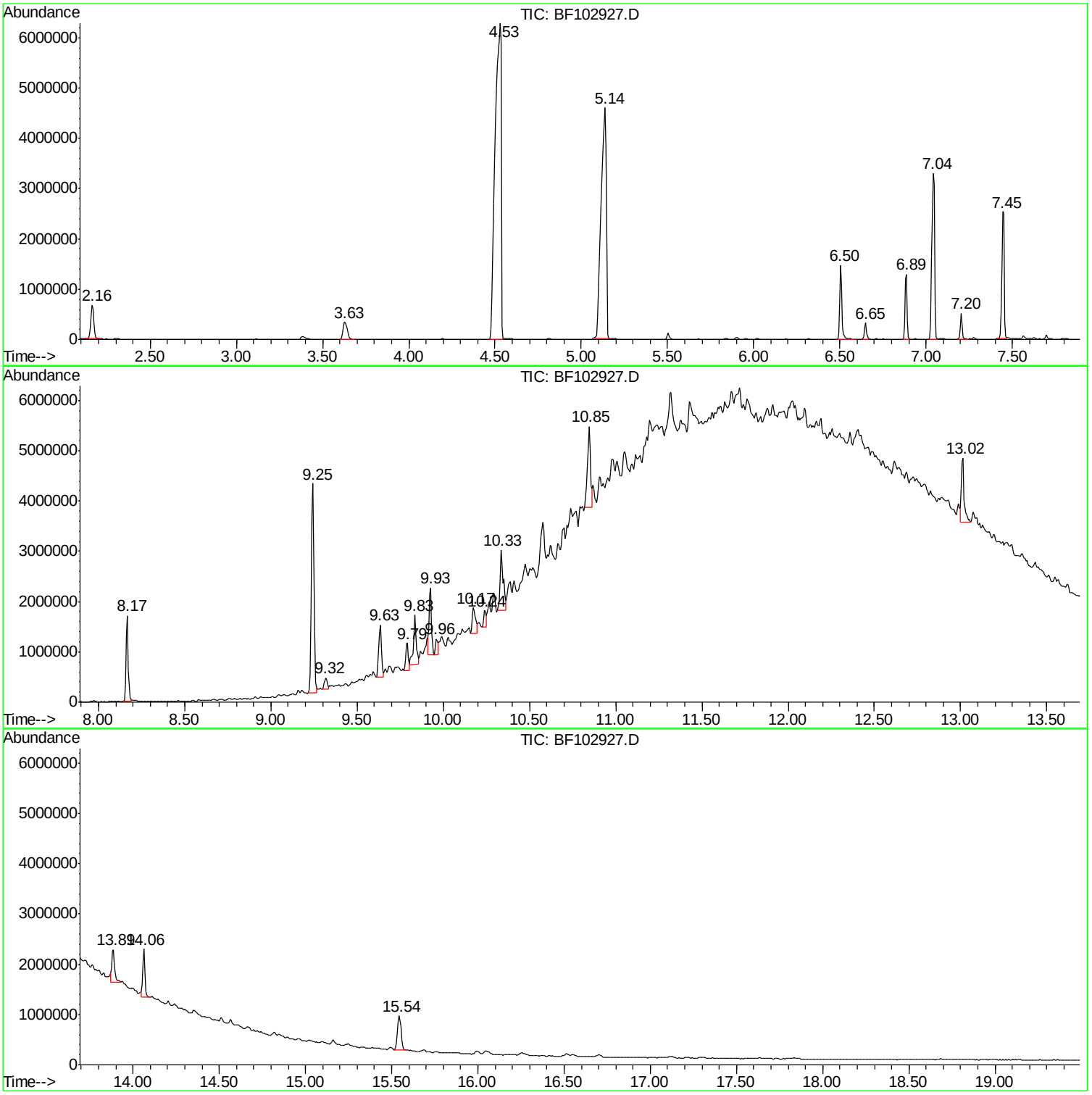
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CO-W

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



Library Search Compound Report

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Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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

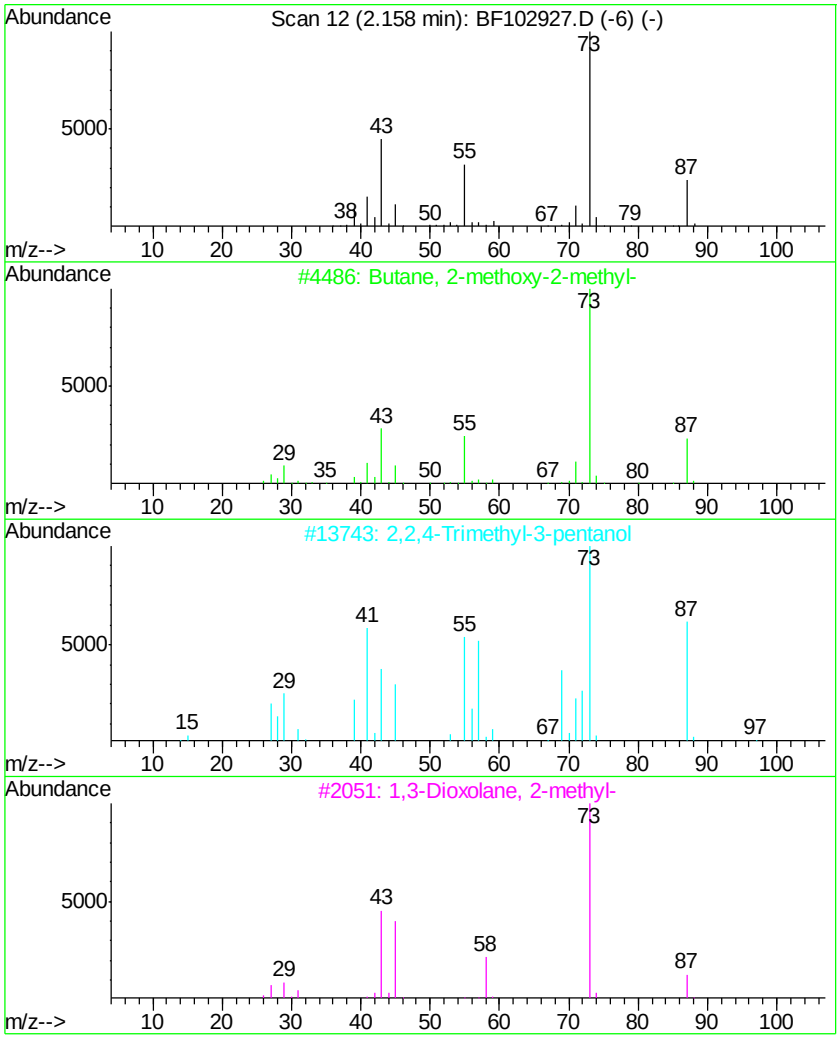
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

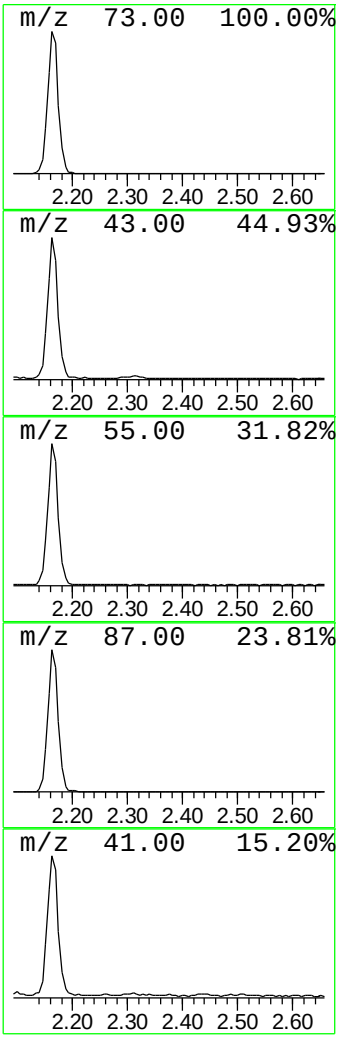
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	15.52 ng	884159	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	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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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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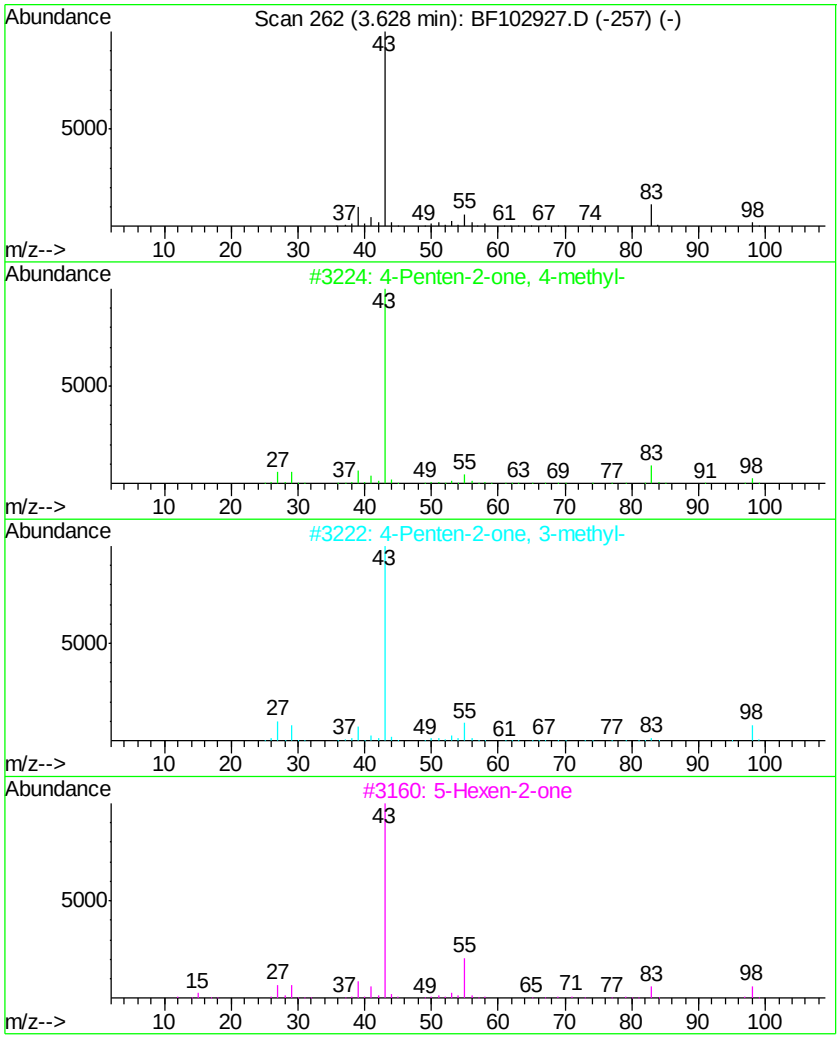
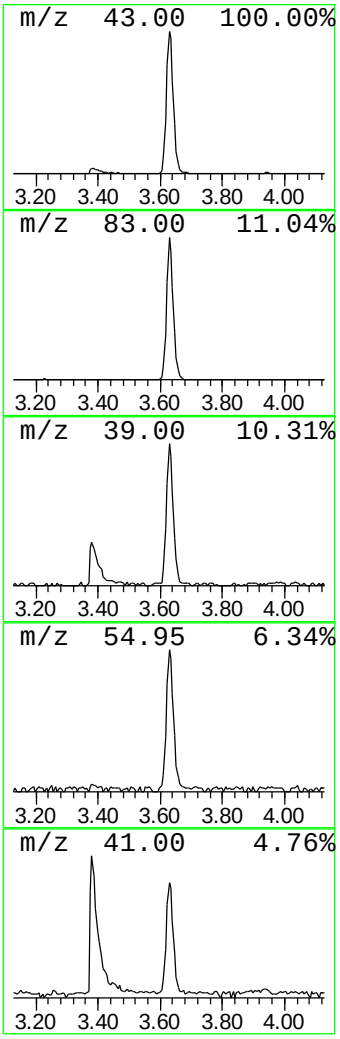
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.63	9.44 ng	537669	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	38
3	5-Hexen-2-one	98	C6H10O	000109-49-9	32
4	4-Hexen-2-one	98	C6H10O	025659-22-7	9
5	2-Vinylethyl acetate	114	C6H10O2	001576-84-7	9





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Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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

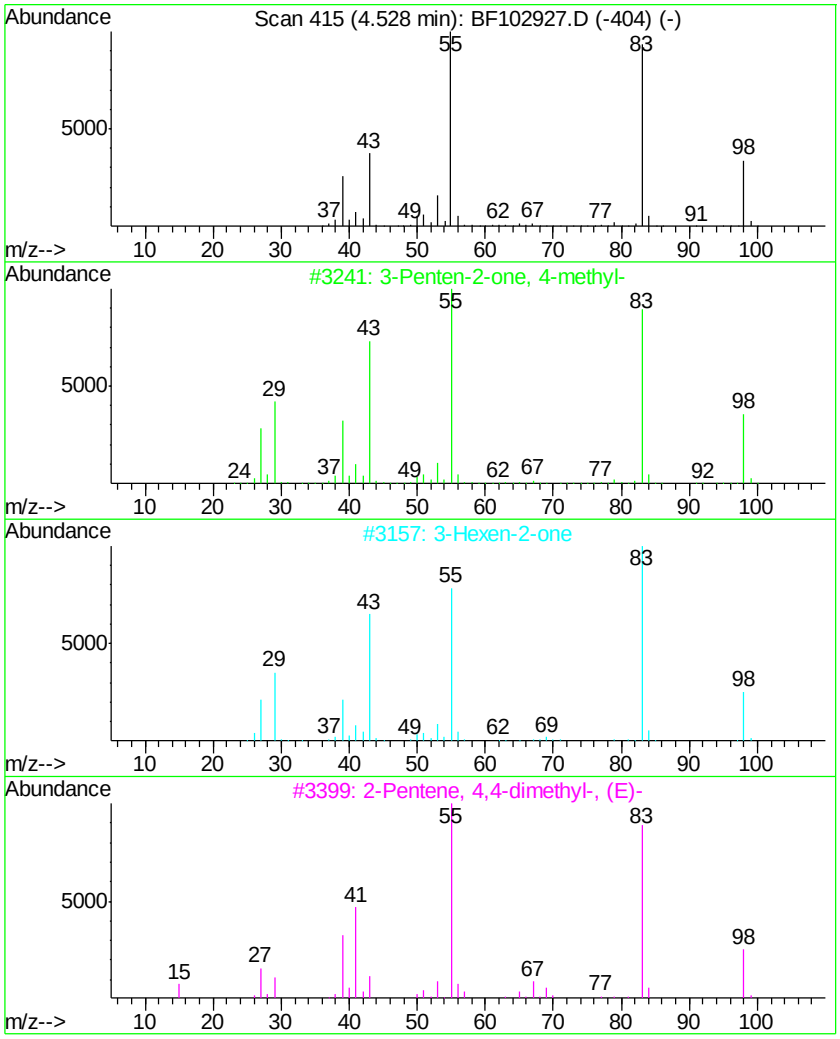
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

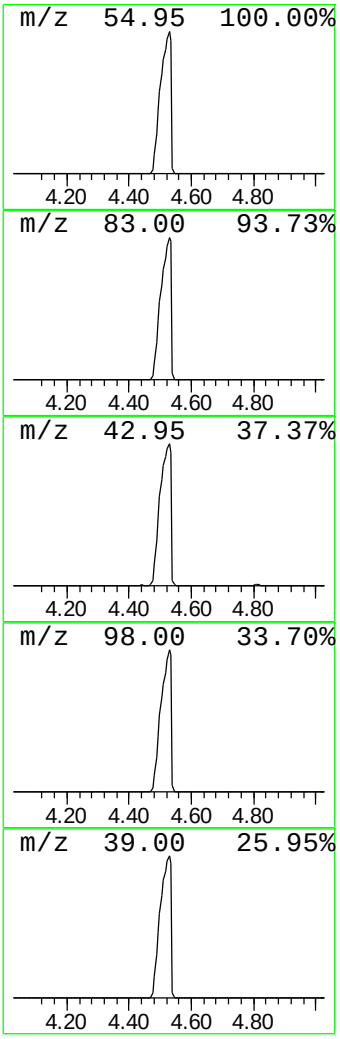
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	262.45 ng	14954200	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





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Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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

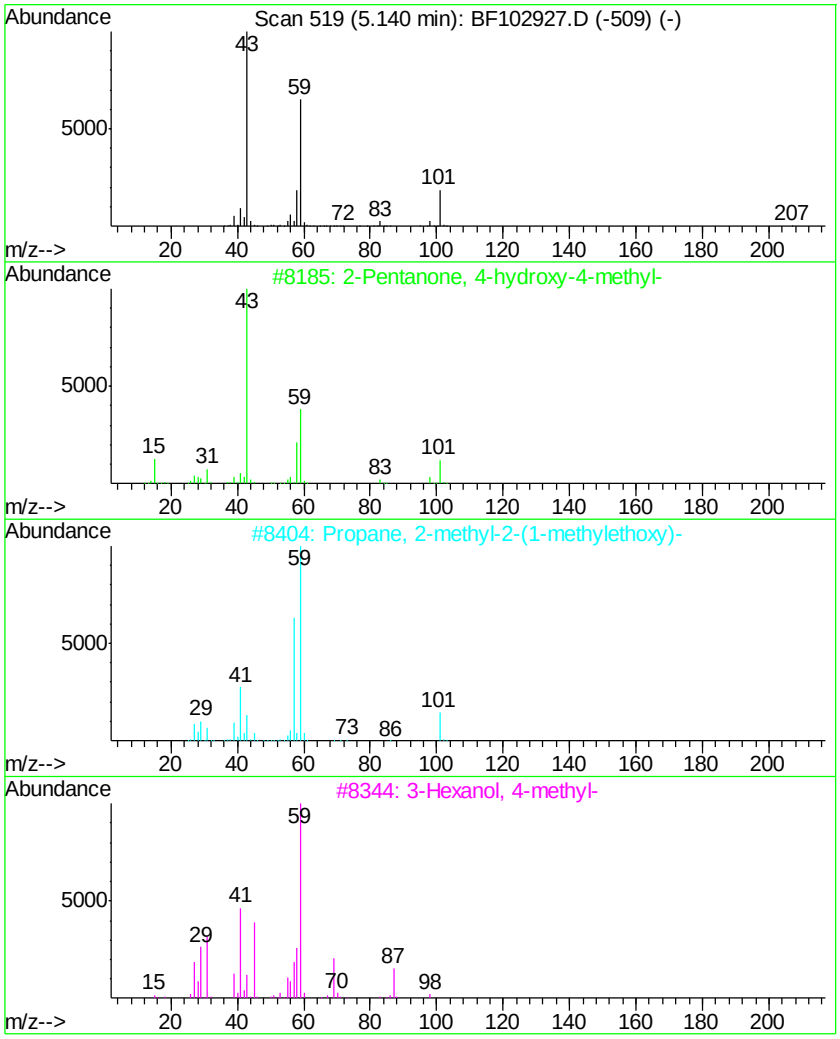
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

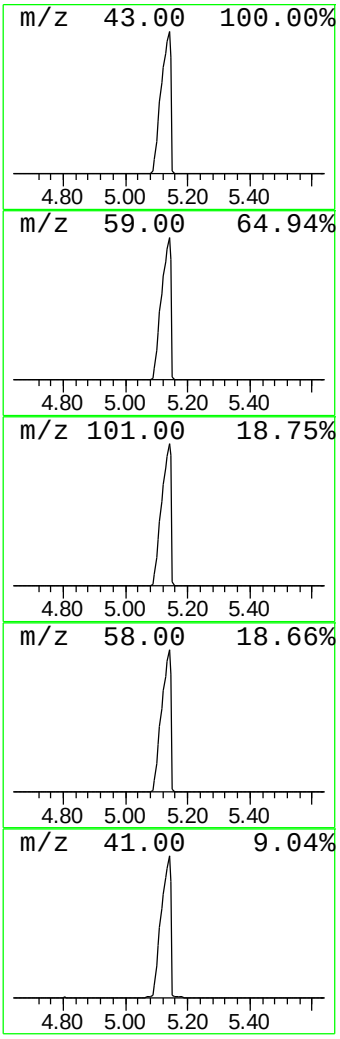
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	173.76 ng	9900440	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	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

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Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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

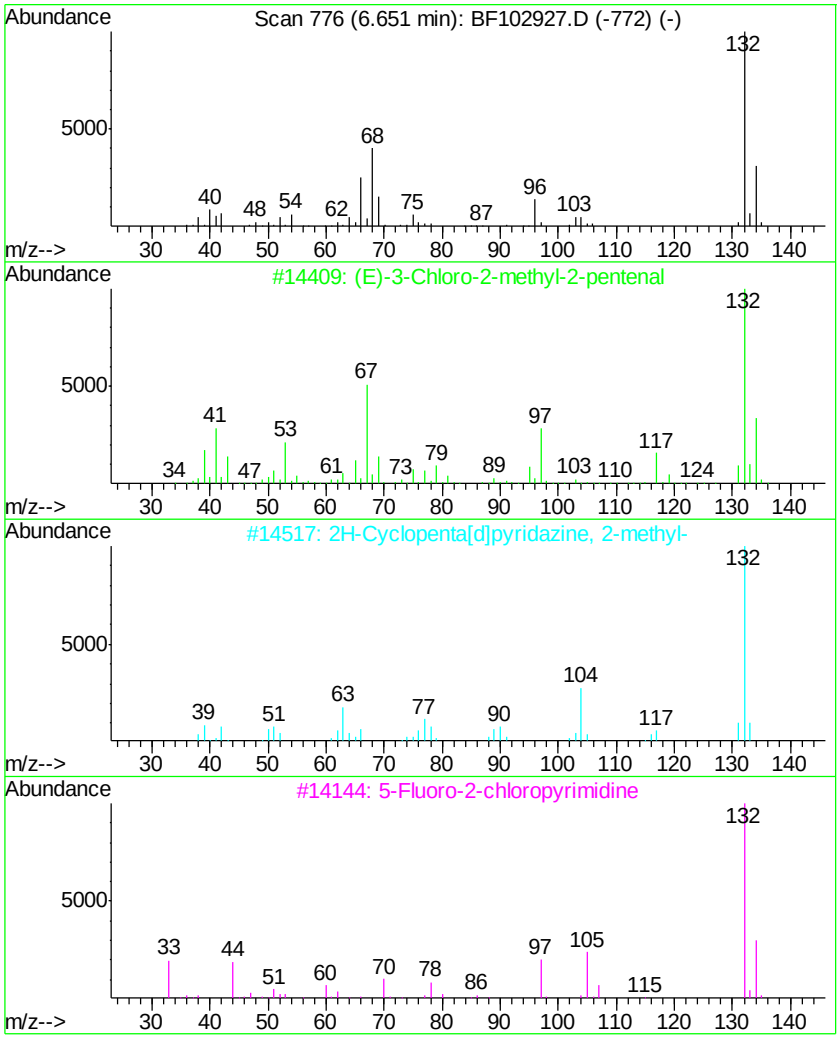
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

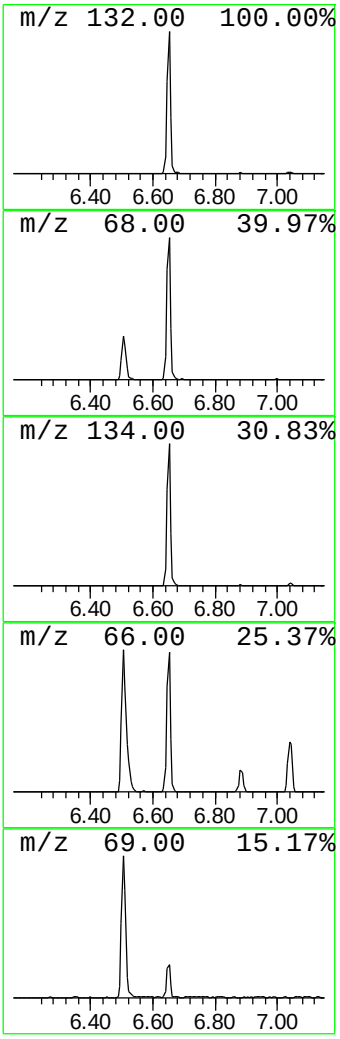
****

Peak Number 5 unknown6.65 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	4.59 ng	261357	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Library Search Compound Report

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Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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

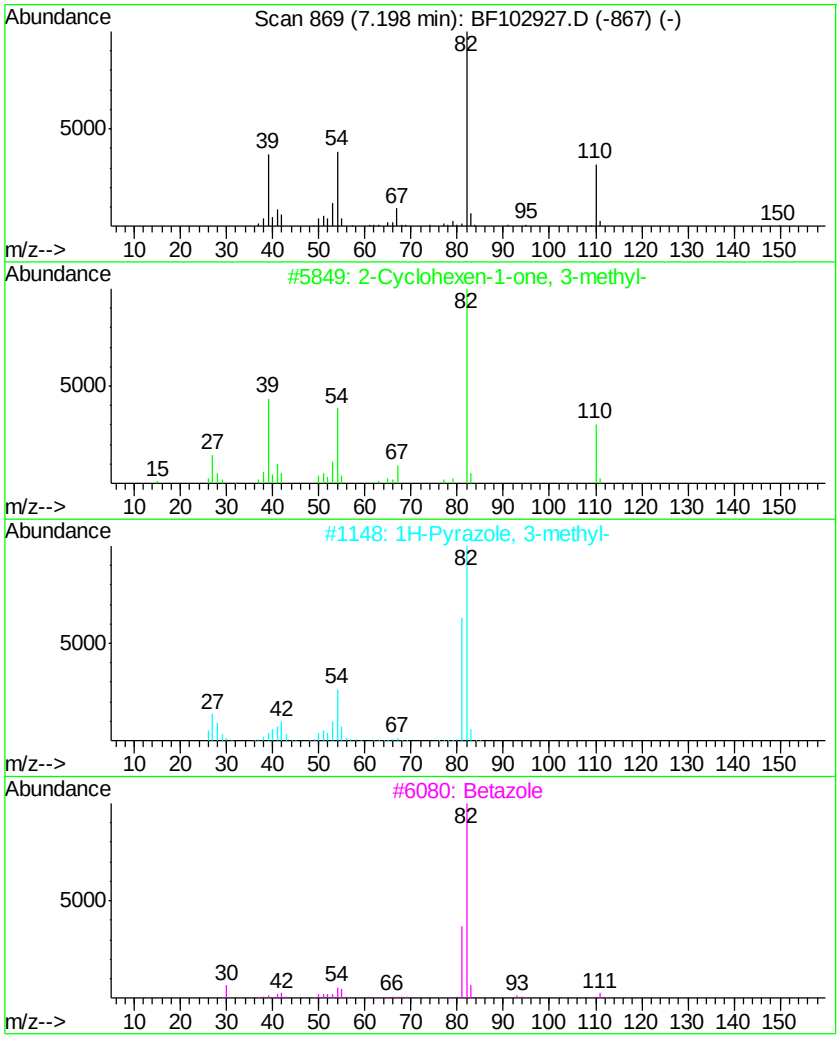
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

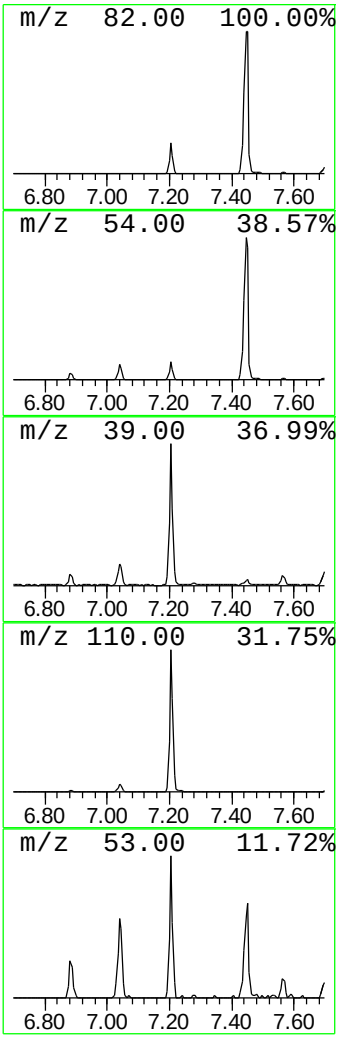
****

Peak Number 7 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	6.96 ng	396352	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	50
3	Betazole	111	C5H9N3	000105-20-4	47
4	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	42
5	1,2,3,6-Tetrahydropyridine	83	C5H9N	000694-05-3	10





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Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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

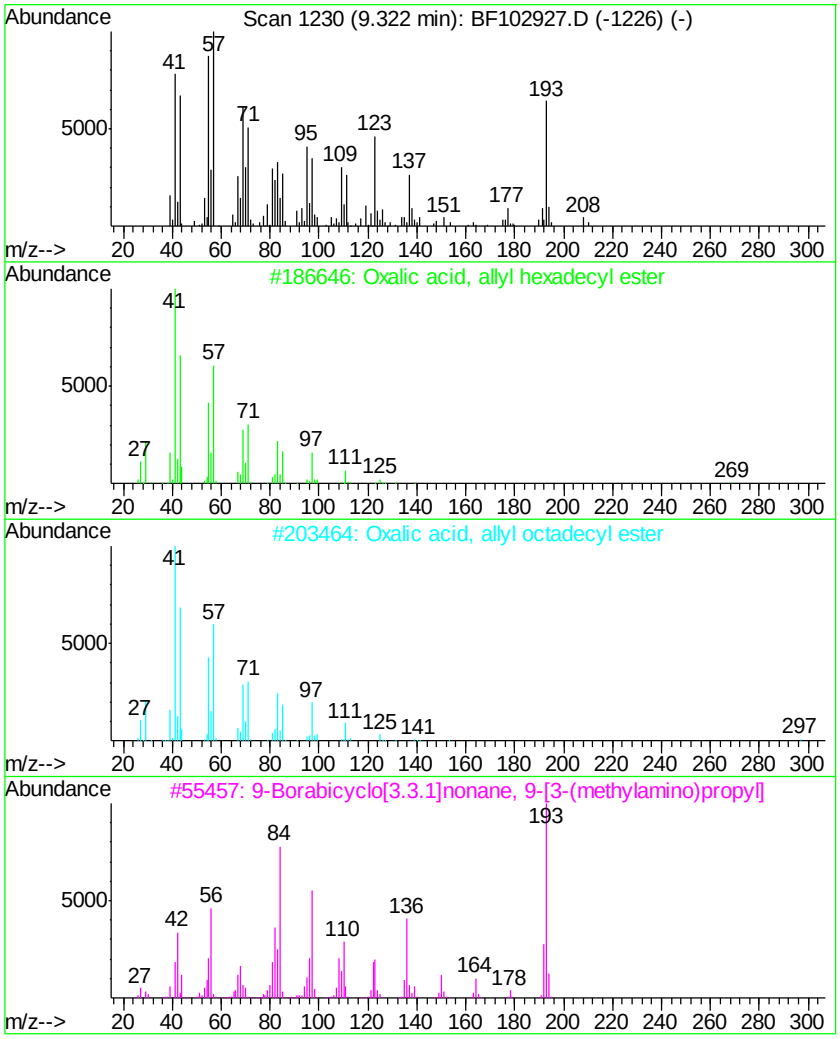
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

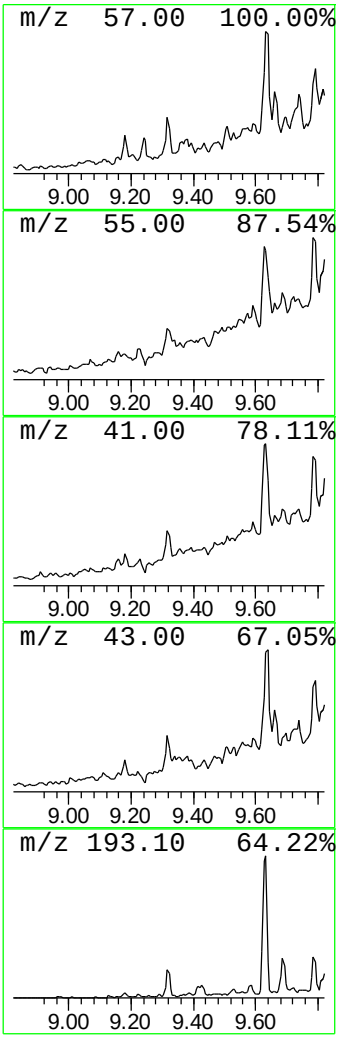
****

Peak Number 8 unknown9.32 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.32	3.94 ng	248668	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	22
2	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	22
3	9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1000162-56-0	18
4	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	18
5	Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	14





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Misc :
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Instrument : BNA_F
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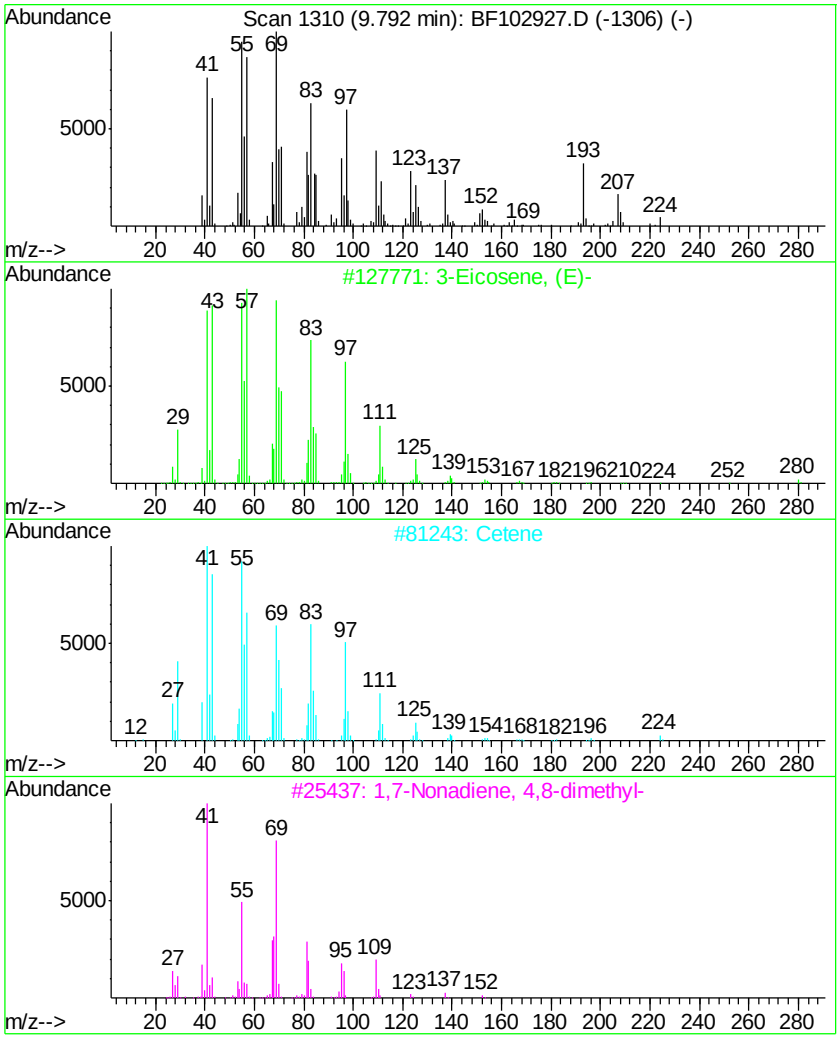
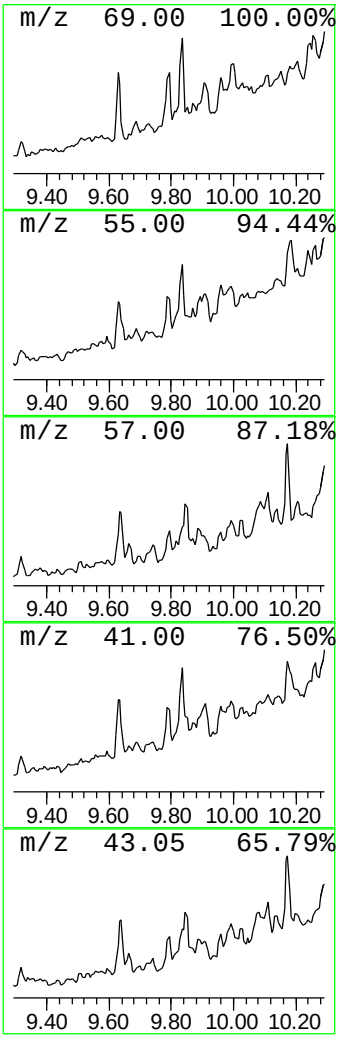
****

Peak Number 9 unknown9.79 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.79	9.60 ng	605741	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	49
2	Cetene	224	C16H32	000629-73-2	44
3	1,7-Nonadiene, 4,8-dimethyl-	152	C11H20	062108-28-5	43
4	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	41
5	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	38





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Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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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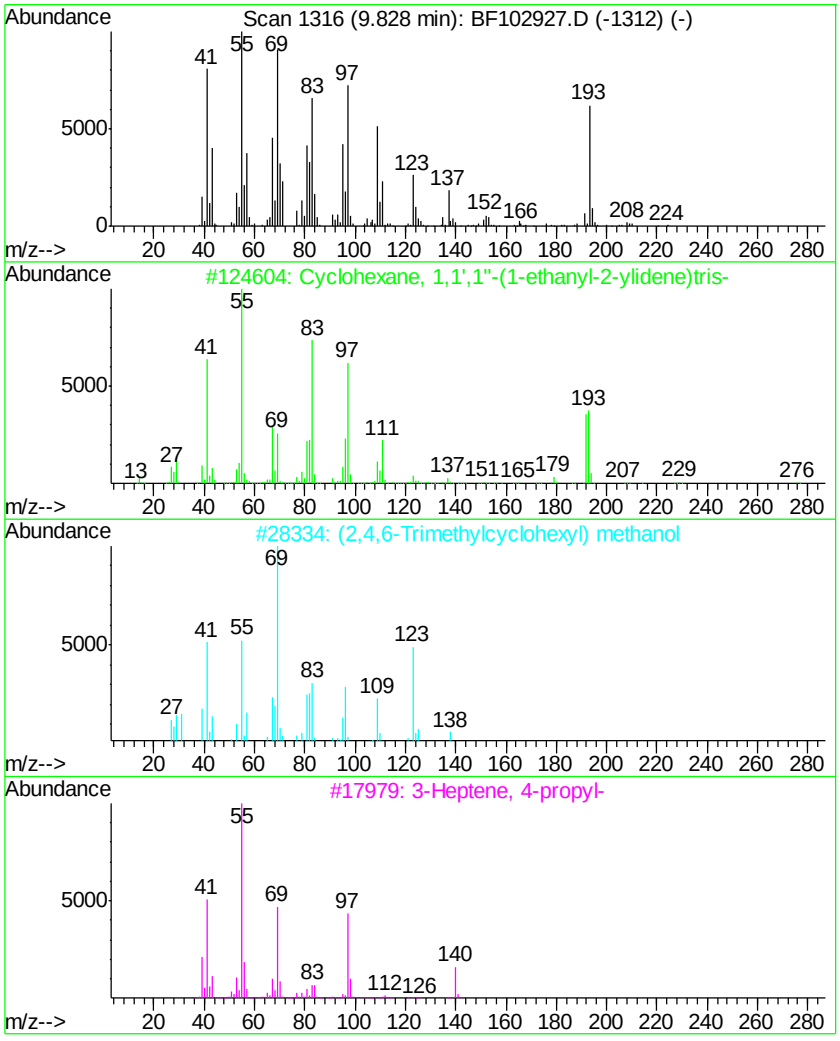
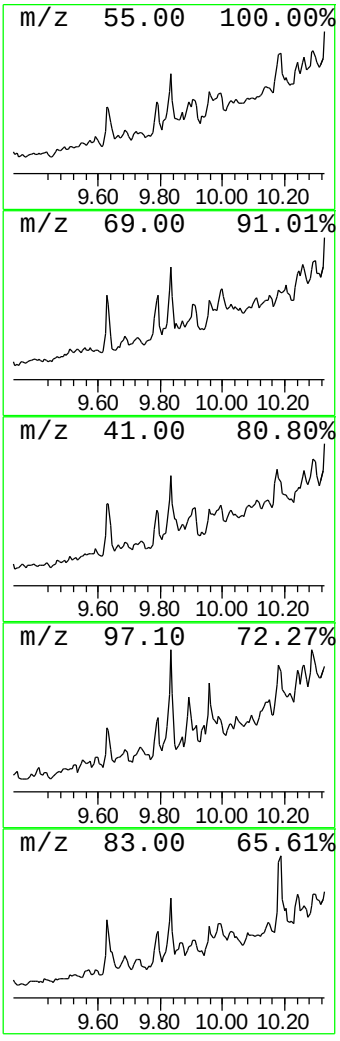
Peak Number 10 unknown9.83 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	18.26 ng	1152870	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	27
2	(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22
3	3-Heptene, 4-propyl-	140	C10H20	004485-13-6	22
4	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-98-2	15
5	(5-Ethylcyclopent-1-enyl)methanol	126	C8H14O	036431-59-1	14





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Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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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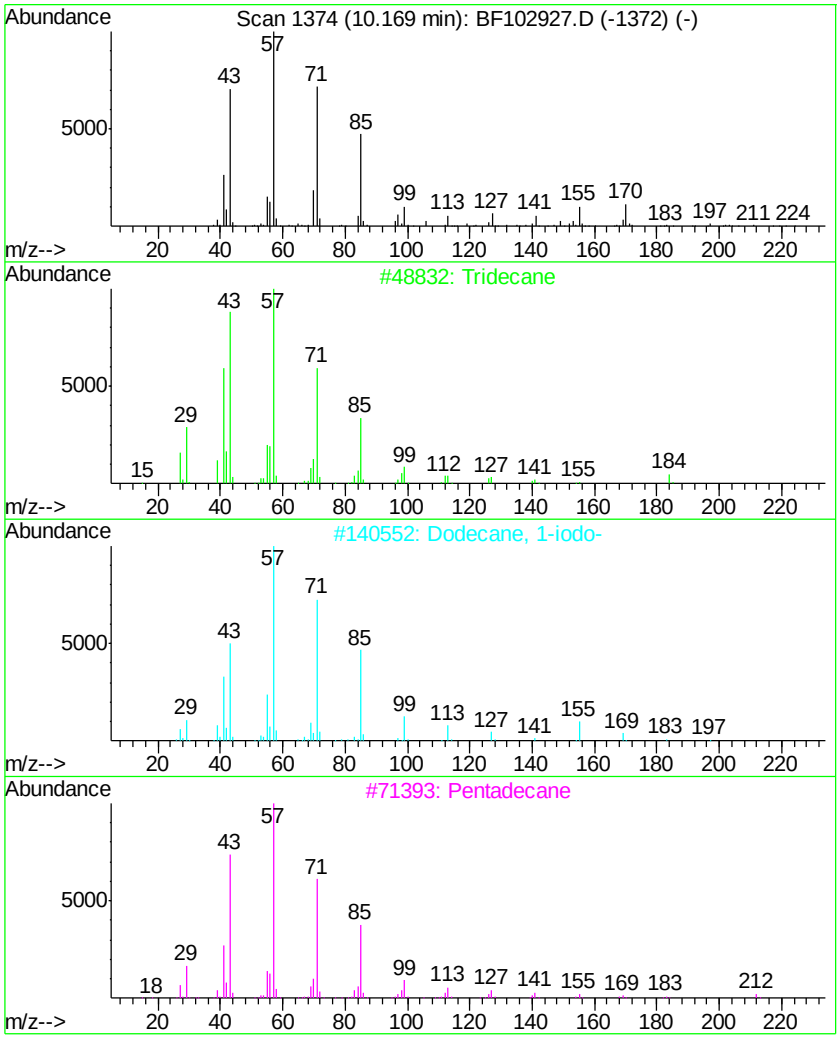
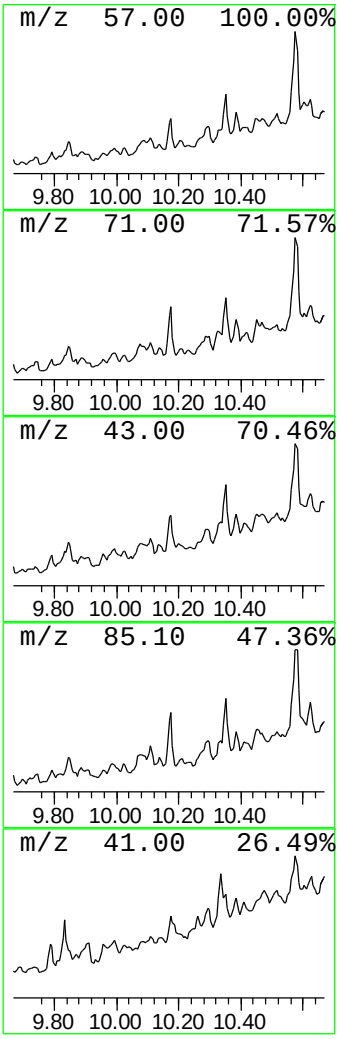
Peak Number 11 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.17	10.35 ng	653355	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
3	Pentadecane	212	C15H32	000629-62-9	64
4	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	59
5	1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	58





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Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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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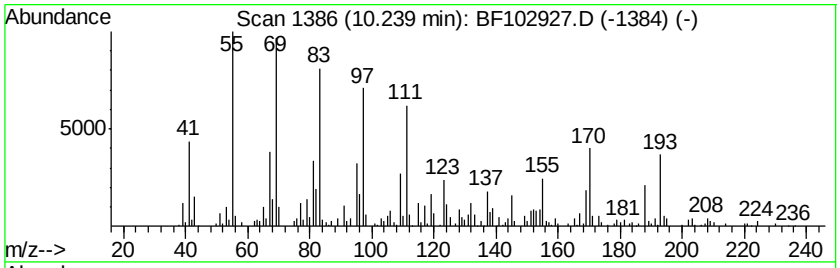
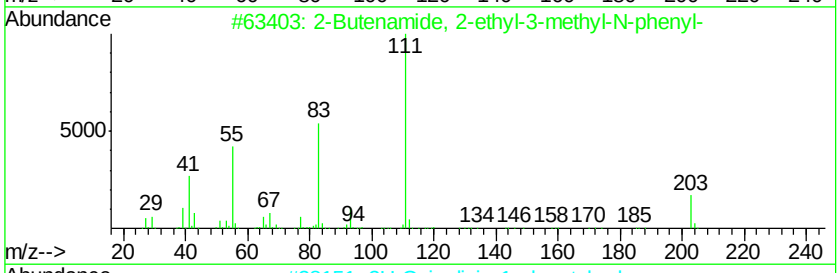
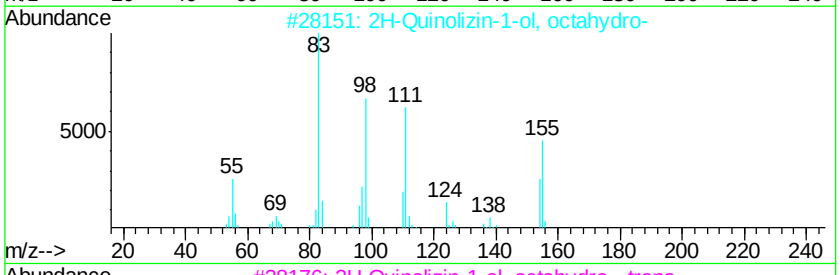
Peak Number 12 unknown10.24 Concentration Rank 13

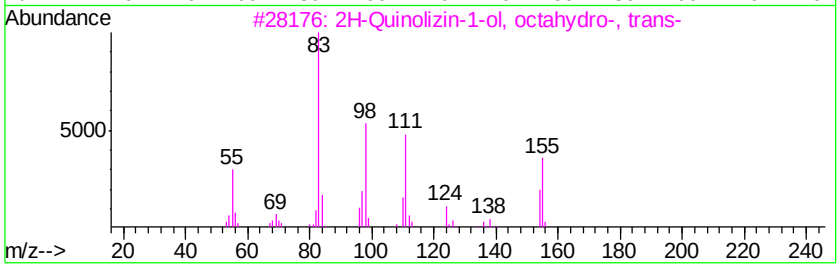
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	5.66 ng	357508	Acenaphthene-d10	9.93

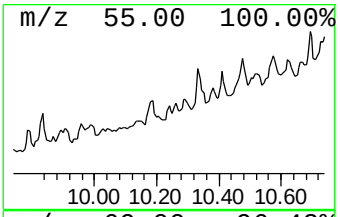
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenamide, 2-ethyl-3-methyl-N...	203	C13H17NO	095383-61-2	35
2	2H-Quinolizin-1-ol, octahydro-	155	C9H17NO	022525-60-6	30
3	2H-Quinolizin-1-ol, octahydro-, ...	155	C9H17NO	010447-20-8	27
4	2H-Quinolizin-1-ol, octahydro-, ...	155	C9H17NO	010447-19-5	22
5	Cyclooctane, cyclohexyl-	194	C14H26	092369-78-3	22

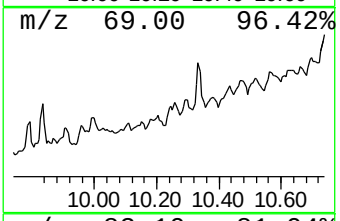


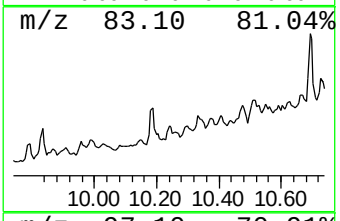


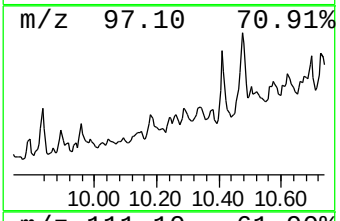


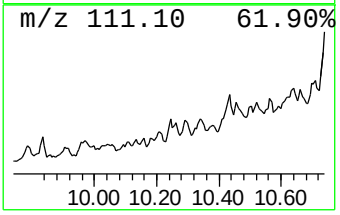












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Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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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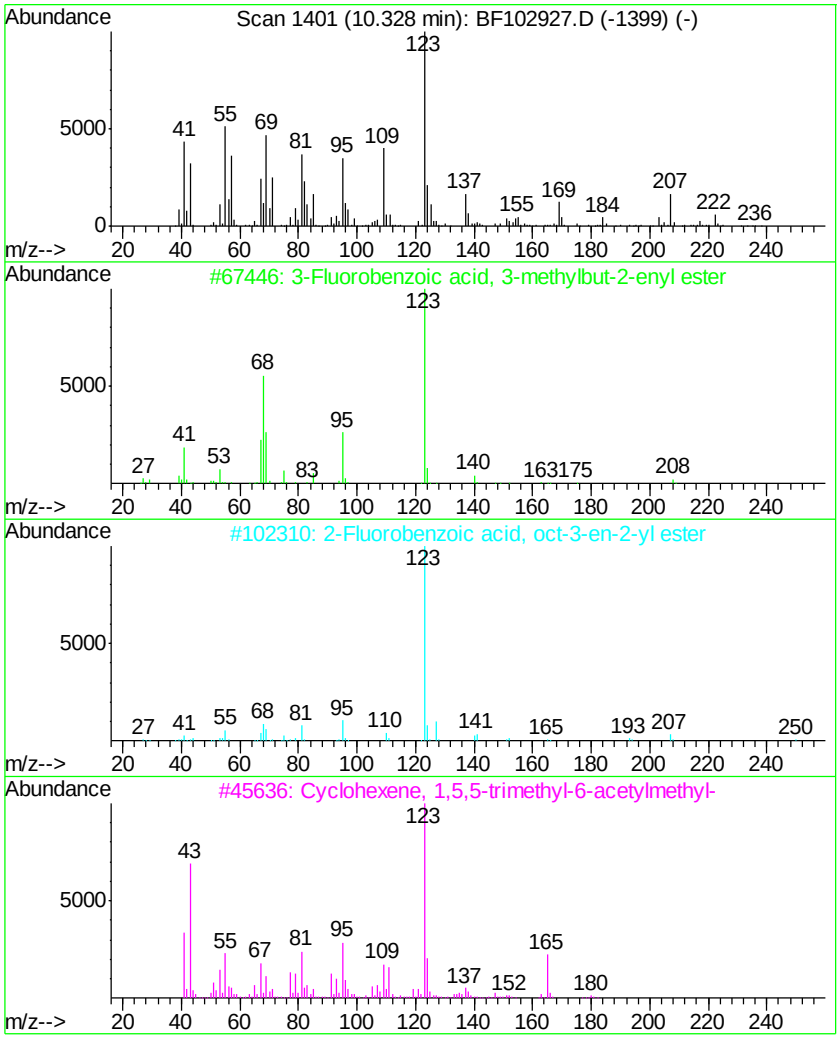
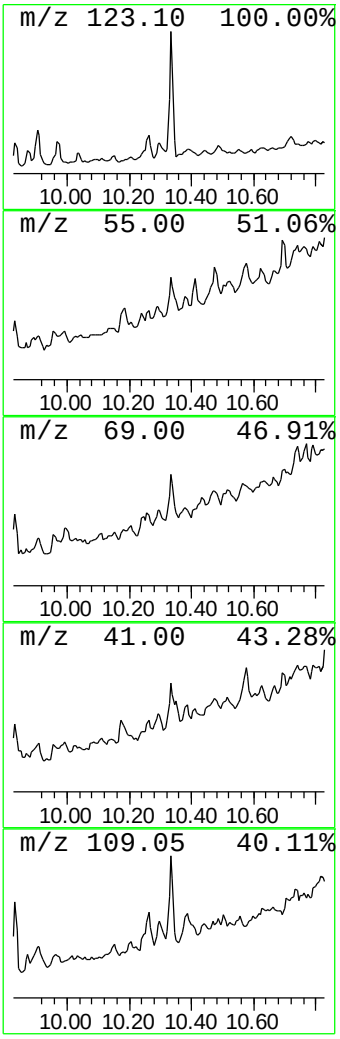
Peak Number 13 unknown10.33 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	25.63 ng	1618070	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	49
2	2-Fluorobenzoic acid, oct-3-en-2...	250	C15H19FO2	1000299-16-5	47
3	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	47
4	2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	47
5	2-(2-Ethyl-1,3-dimethyl-cyclopen...	182	C12H22O	1000186-82-4	43





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Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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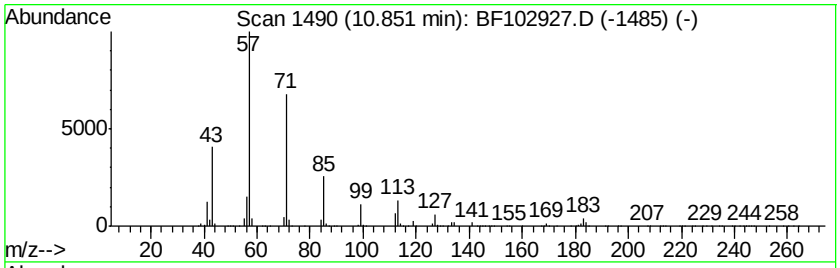
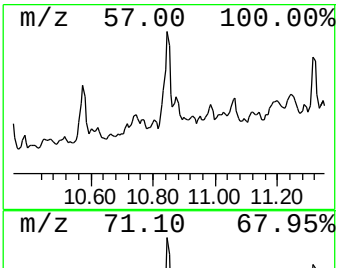
Peak Number 14 Tridecane, 6-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	20.00 ng	2127070	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 6-methyl-	198	C14H30	013287-21-3	74
2	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	53
3	Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	53
4	Tridecane, 7-methyl-	198	C14H30	026730-14-3	52
5	Dodecane, 2,5-dimethyl-	198	C14H30	056292-65-0	52





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Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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TIC Integration Parameters: LSCINT.P

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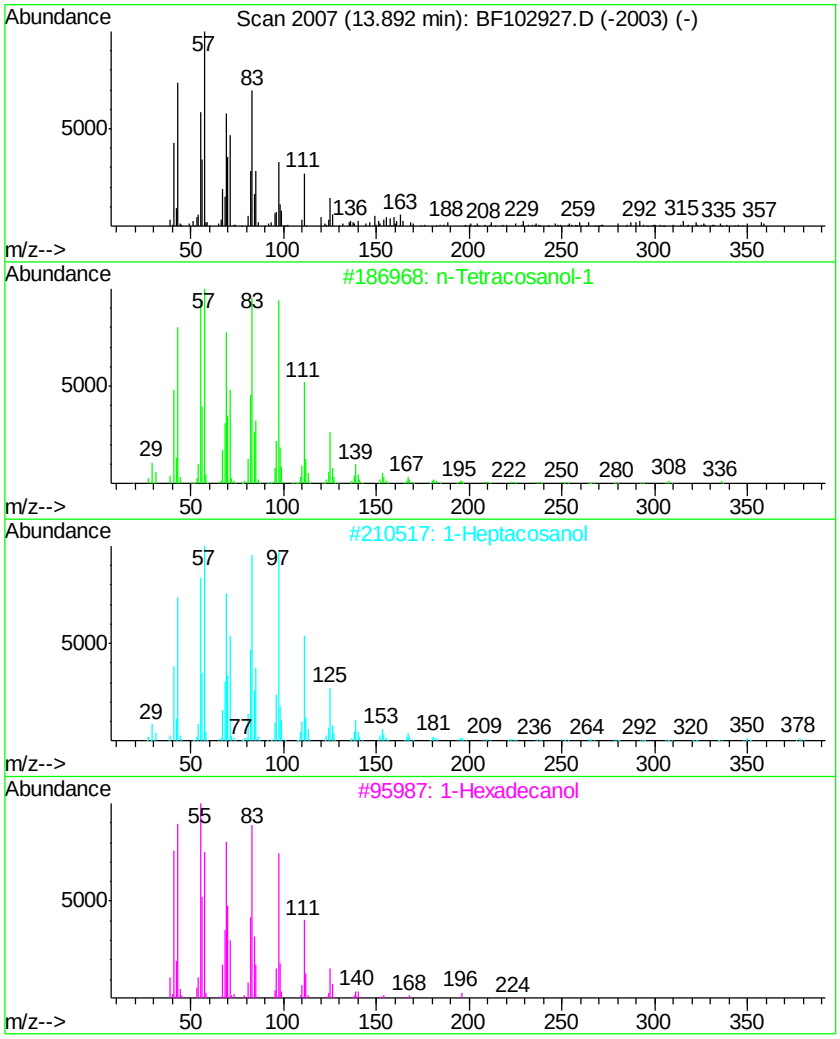
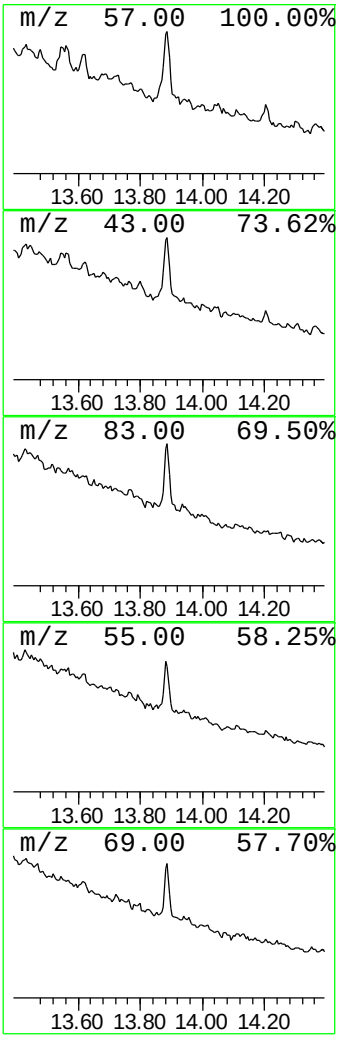
Peak Number 15 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	17.08 ng	772018	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	87
3	1-Hexadecanol	242	C16H34O	036653-82-4	83
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	78
5	5-Methyl-Z-5-docosene	322	C23H46	1000131-17-1	76





Tentatively Identified Compound (LSC) summary

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Data File : BF102927.D
Acq On : 12 Feb 2018 18:17
Operator : SJ/JU
Sample : J1517-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-W

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...	2.16	15.5	ng	884159	1	6.89	1139570	20.0
4-Penten-2-one, 4...	3.63	9.4	ng	537669	1	6.89	1139570	20.0
3-Penten-2-one, 4...	4.53	262.4	ng	14954200	1	6.89	1139570	20.0
2-Pentanone, 4-hy...	5.14	173.8	ng	9900440	1	6.89	1139570	20.0
unknown6.65	6.65	4.6	ng	261357	1	6.89	1139570	20.0
2-Cyclohexen-1-on...	7.20	7.0	ng	396352	1	6.89	1139570	20.0
unknown9.32	9.32	3.9	ng	248668	3	9.93	1262440	20.0
unknown9.79	9.79	9.6	ng	605741	3	9.93	1262440	20.0
unknown9.83	9.83	18.3	ng	1152870	3	9.93	1262440	20.0
Tridecane	10.17	10.4	ng	653355	3	9.93	1262440	20.0
unknown10.24	10.24	5.7	ng	357508	3	9.93	1262440	20.0
unknown10.33	10.33	25.6	ng	1618070	3	9.93	1262440	20.0
Tridecane, 6-methyl-	10.85	20.0	ng	2127070	4	11.43	2127070	20.0
n-Tetracosanol-1	13.89	17.1	ng	772018	5	14.06	904190	20.0