LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097169.D
Acq On : 28 Jul 2017 22:22
Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

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-BF072517.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	4.634	463	467	484	rBV	552886	867230	28.29%	3.512%
2	5.093	540	545	558	rBV	2765352	3065423	100.00%	12.414%
3	6.157	721	726	740	rBV	2635229	3018432	98.47%	12.224%
4	6.263	740	744	757	rVB	2904143	2793264	91.12%	11.312%
5	6.487	778	782	786	rBV	890740	752546	24.55%	3.048%
6	6.522	786	788	794	rVB2	26935	37943	1.24%	0.154%
7	6.645	804	809	812	rBV	1951748	1937779	63.21%	7.847%
8	6.692	815	817	825	rVB	23143	39867	1.30%	0.161%
9	7.057	874	879	882	rBV	1824680	1703565	55.57%	6.899%
10	7.198	898	903	909	rVB	39170	43507	1.42%	0.176%
11	7.510	952	956	960	rVB	33127	33488	1.09%	0.136%
12	7.698	983	988	992	rBV	27075	33399	1.09%	0.135%
13	7.769	996	1000	1005	rBV	1154245	971049	31.68%	3.932%
14	8.851	1179	1184	1187	rBV	2309200	2290565	74.72%	9.276%
15	9.245	1248	1251	1256	rBV	498111	394112	12.86%	1.596%
16	9.516	1293	1297	1301	rBV	987557	892964	29.13%	3.616%
17	9.751	1334	1337	1341	rBV	34998	34016	1.11%	0.138%
18	9.969	1371	1374	1377	rVB	48045	37362	1.22%	0.151%
19	10.298	1427	1430	1443	rVB	1208222	1198710	39.10%	4.854%
20	10.439	1451	1454	1462	rBV	71433	81598	2.66%	0.330%
21	10.886	1526	1530	1532	rBV	48923	44349	1.45%	0.180%
22	10.986	1543	1547	1556	rBV	698744	616941	20.13%	2.498%
23	11.239	1587	1590	1596	rBV	173993	171127	5.58%	0.693%
24	11.545	1639	1642	1644	rBV	56546	58149	1.90%	0.235%
25	11.839	1689	1692	1695	rBV	70399	65794	2.15%	0.266%
26	12.051	1725	1728	1734	rVB2	73013	75388	2.46%	0.305%
27	12.569	1812	1816	1820	rVB	1569925	1584534	51.69%	6.417%
28	12.704	1835	1839	1842	rBV	236630	198456	6.47%	0.804%
29	13.480	1968	1971	1982	rBV	170633	199412	6.51%	0.808%
30	13.610	1989	1993	1997	rBV	703142	640867	20.91%	2.595%
31	14.116	2075	2079	2083	rBV2	59477	70534	2.30%	0.286%
32	14.380	2121	2124	2127	rBV4	28993	44919	1.47%	0.182%
33	14.963	2218	2223	2227	rBV	451686	511334	16.68%	2.071%
34	15.004	2228	2230	2237	rVB2	33561	46724	1.52%	0.189%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097169.D
Acq On : 28 Jul 2017 22:22
Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.363	2288	2291	2294	rBV2	28062	36130	1.18%	0.146%
36	15.774	2357	2361	2366	rBV3	33404	51525	1.68%	0.209%
37	16.245	2439	2441	2450	rVB8	26248	50130	1.64%	0.203%

Sum of corrected areas: 24693132

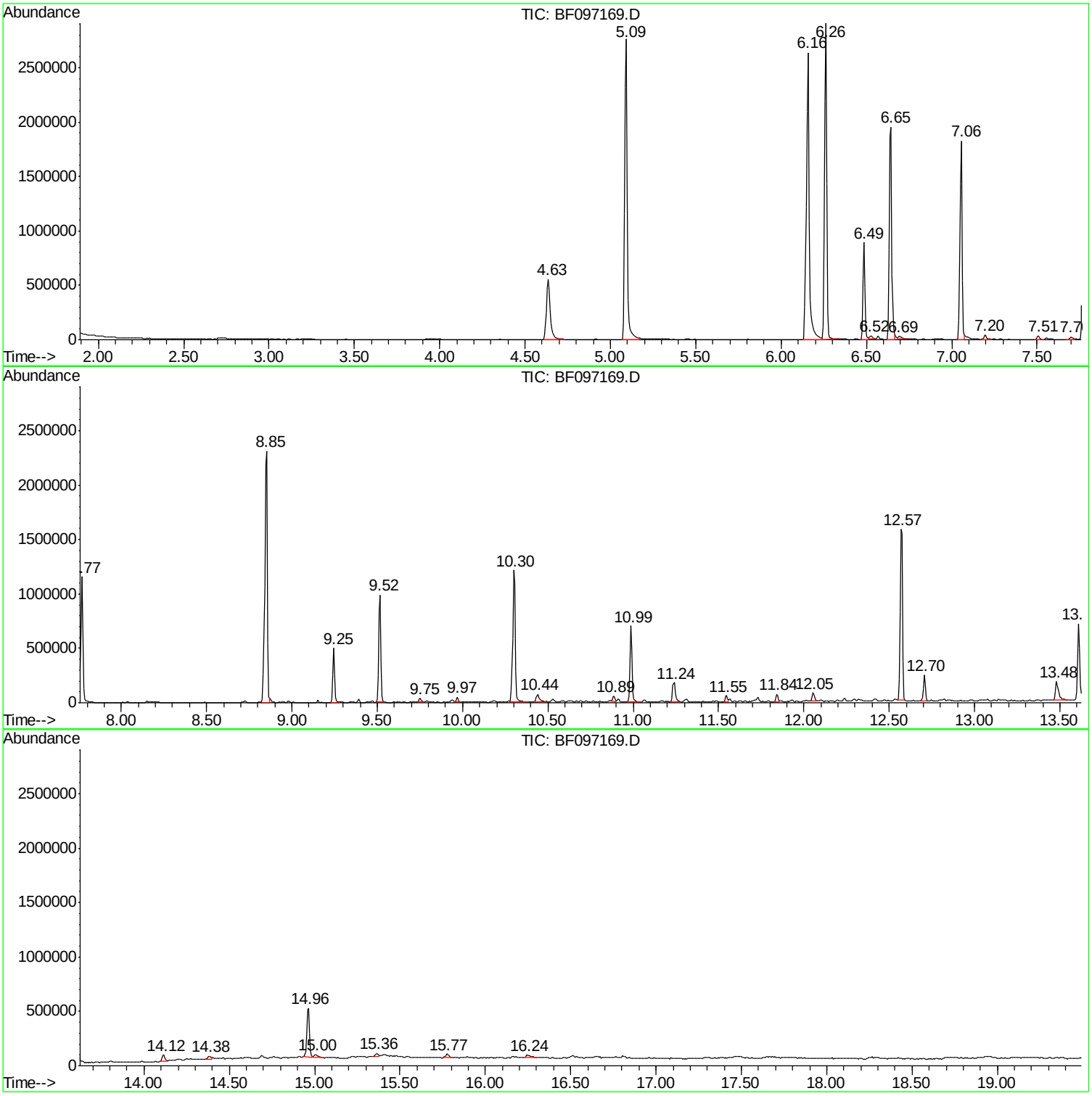
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097169.D
Acq On : 28 Jul 2017 22:22
Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097169.D
Acq On : 28 Jul 2017 22:22
Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

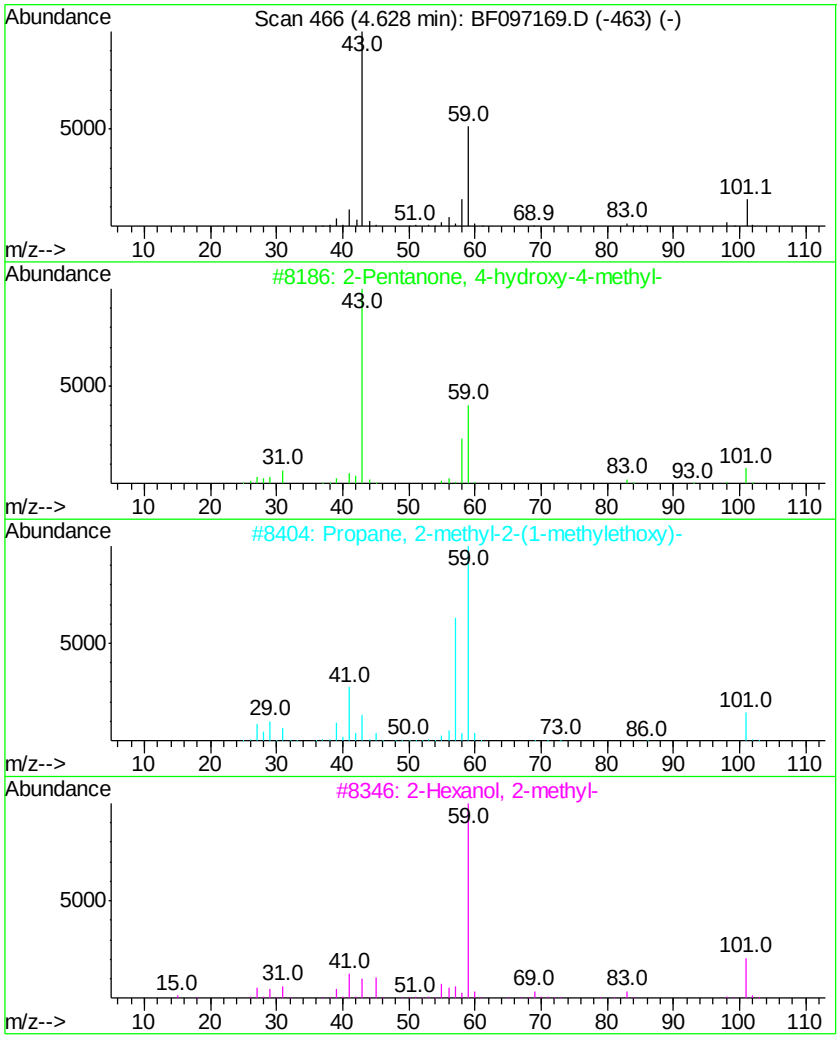
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

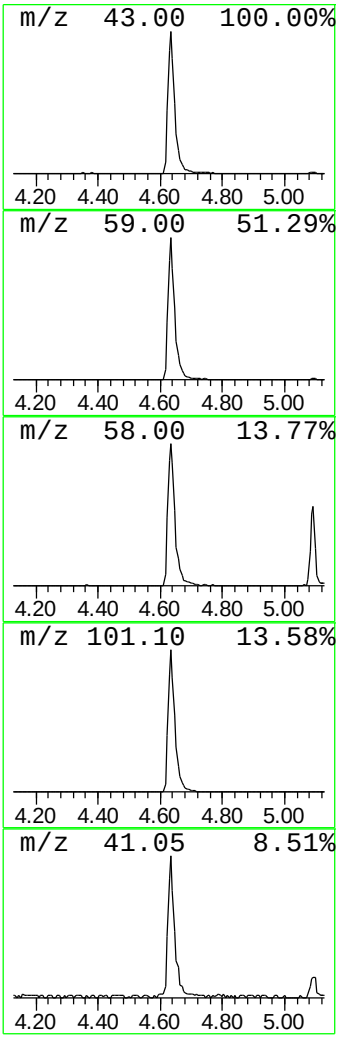
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	23.05 ng	867230	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

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Data File : BF097169.D
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Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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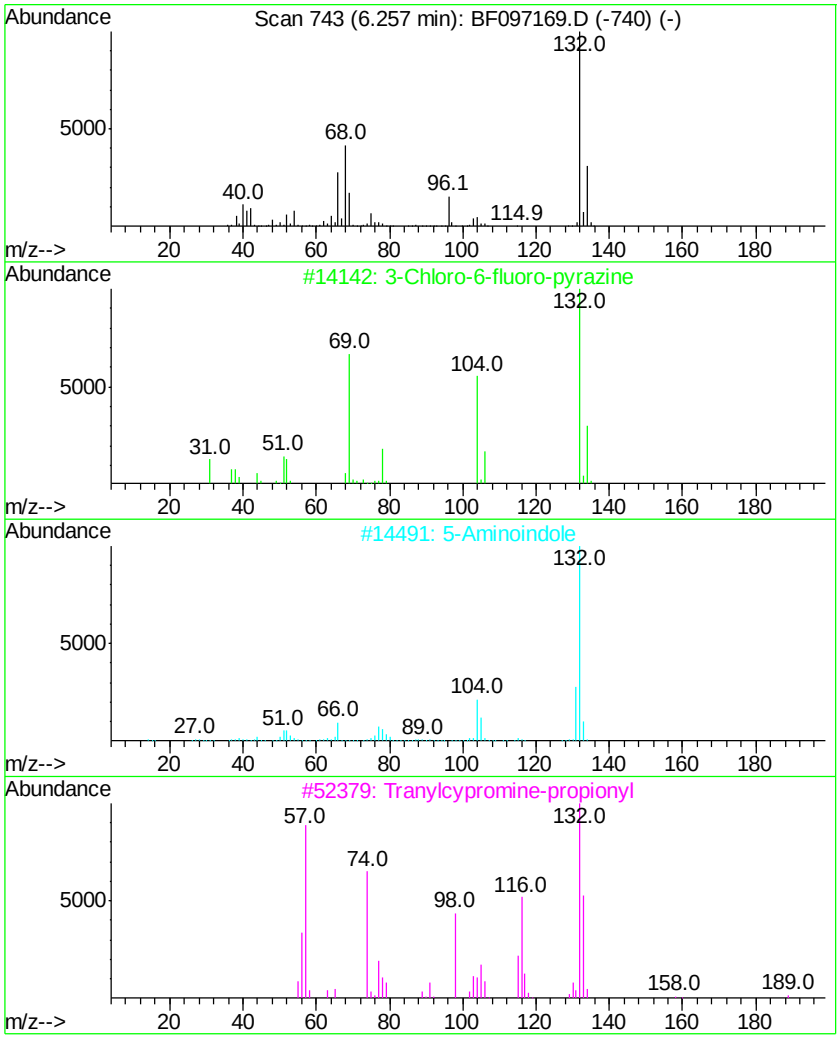
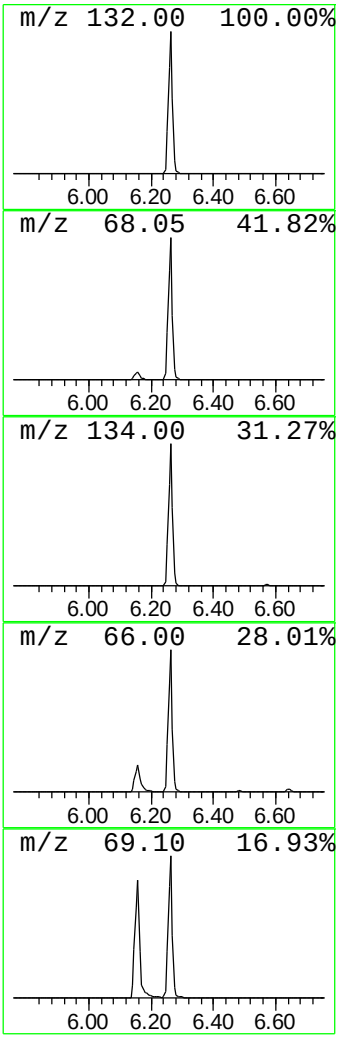
Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	74.24 ng	2793260	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097169.D
Acq On : 28 Jul 2017 22:22
Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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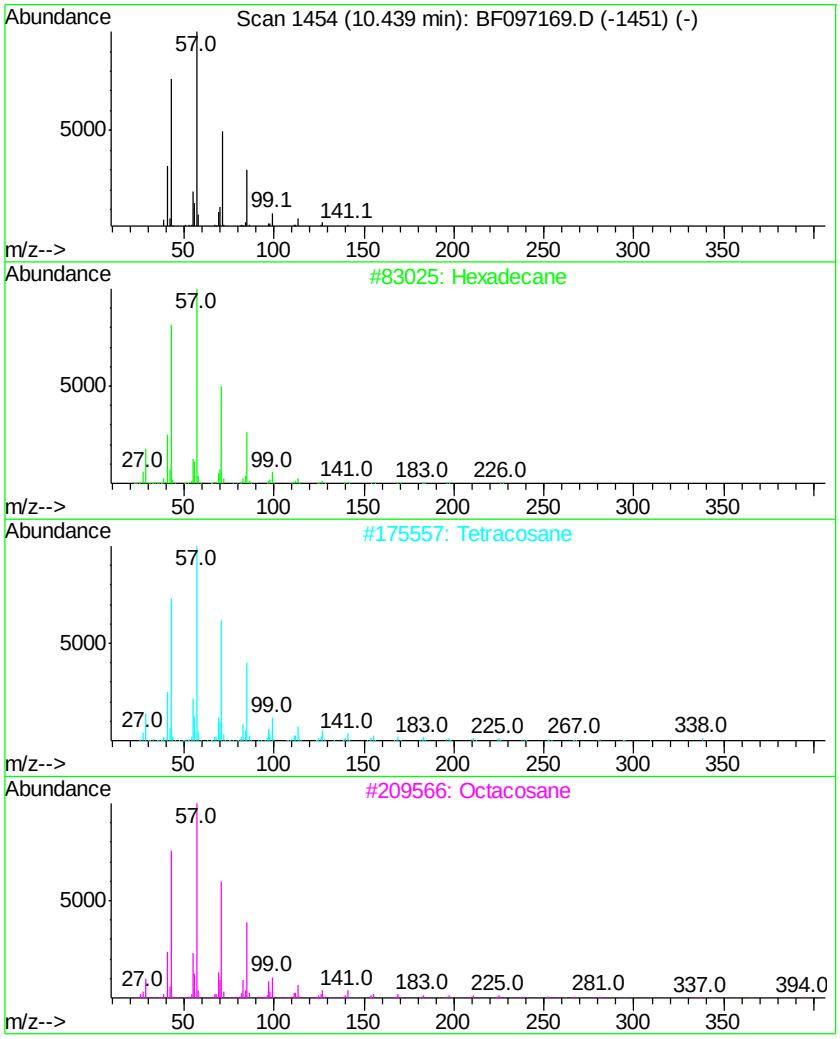
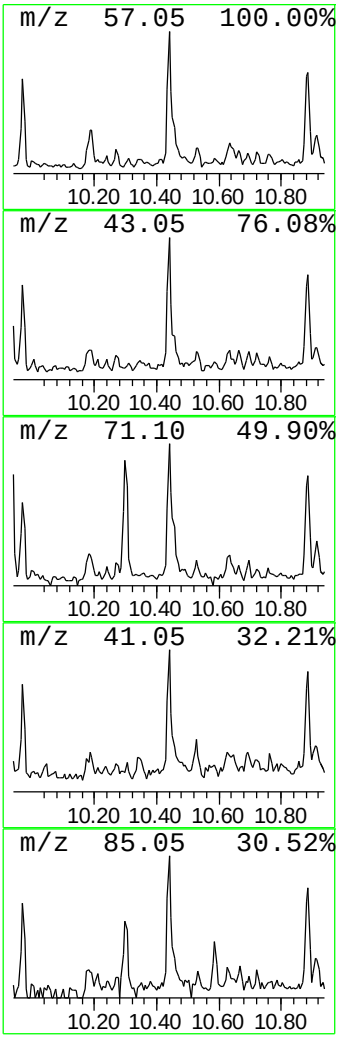
Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.65 ng	81598	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Eicosane	282	C20H42	000112-95-8	86
5	Heneicosane	296	C21H44	000629-94-7	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097169.D
Acq On : 28 Jul 2017 22:22
Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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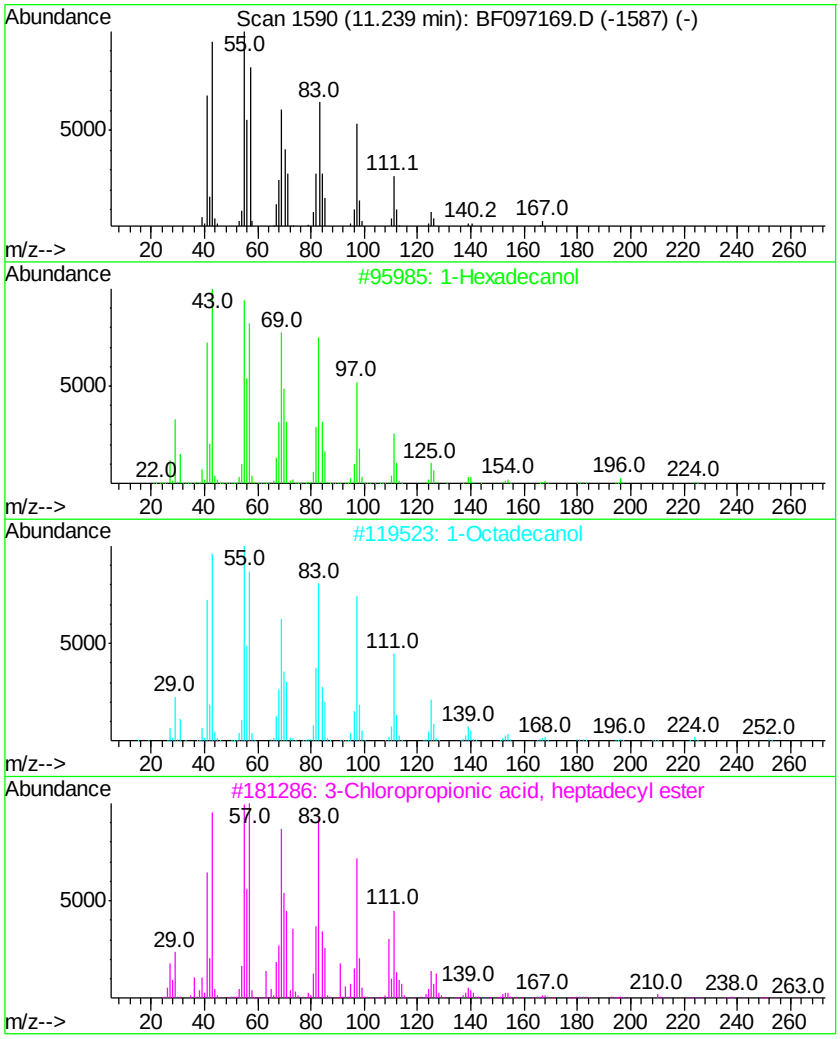
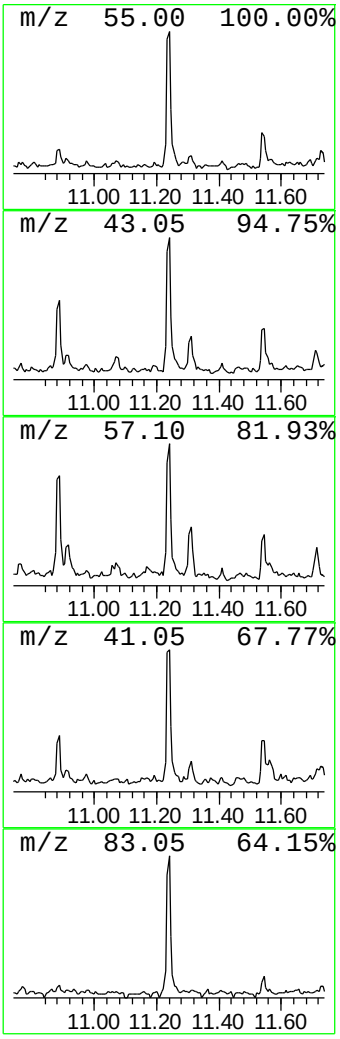
Peak Number 5 1-Hexadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	5.55 ng	171127	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	1-Octadecanol	270	C18H38O	000112-92-5	91
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097169.D
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Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

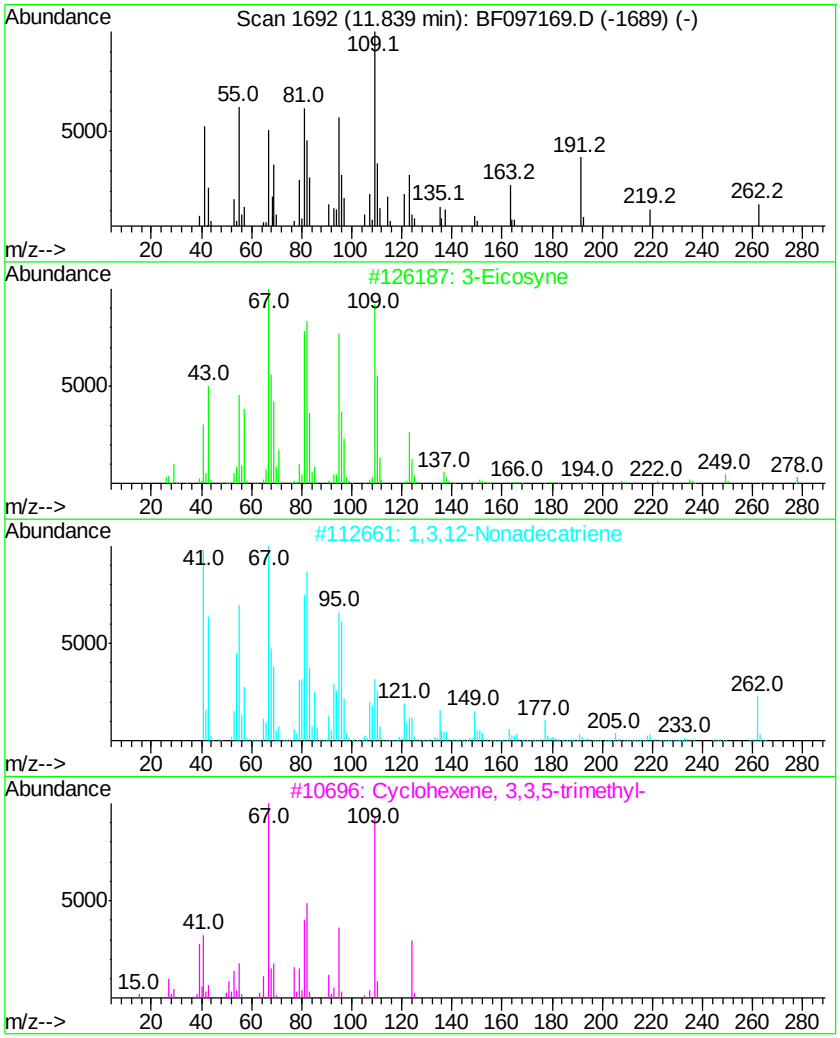
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

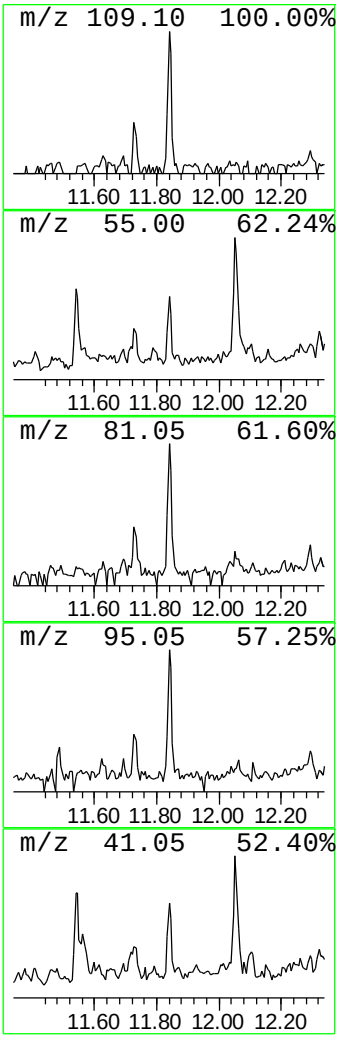
****

Peak Number 6 3-Eicosyne Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.13 ng	65794	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosyne	278	C20H38	061886-66-6	49
2	1,3,12-Nonadecatriene	262	C19H34	1000131-11-1	42
3	Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	41
4	3-Dodecyne	166	C12H22	006790-27-8	38
5	7-Octadecyne, 2-methyl-	264	C19H36	035354-38-2	35





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Data File : BF097169.D
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Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

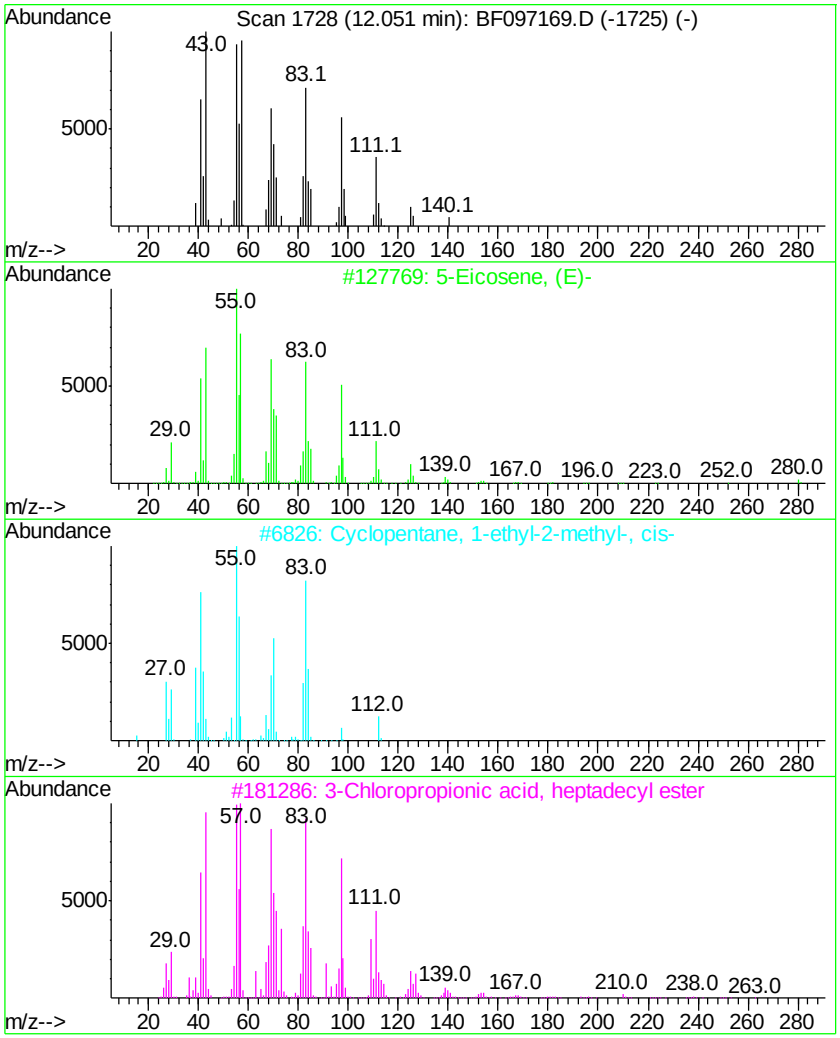
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

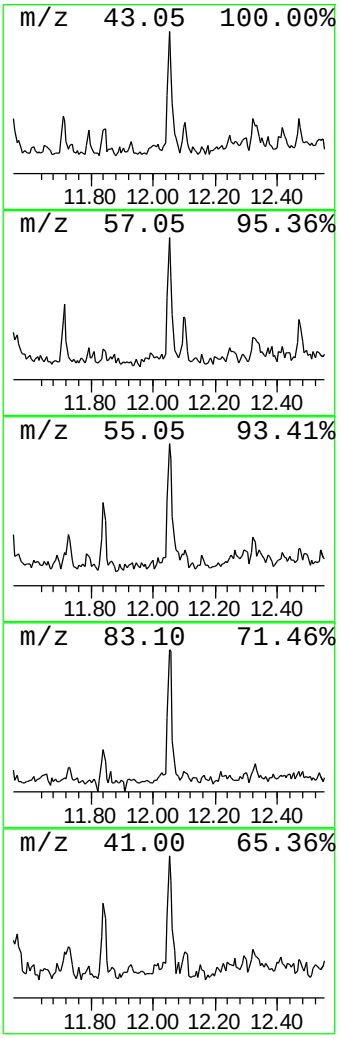
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	2.44 ng	75388	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2	Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	90
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90
4	Cetene	224	C16H32	000629-73-2	87
5	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	87





Library Search Compound Report

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Instrument :
BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

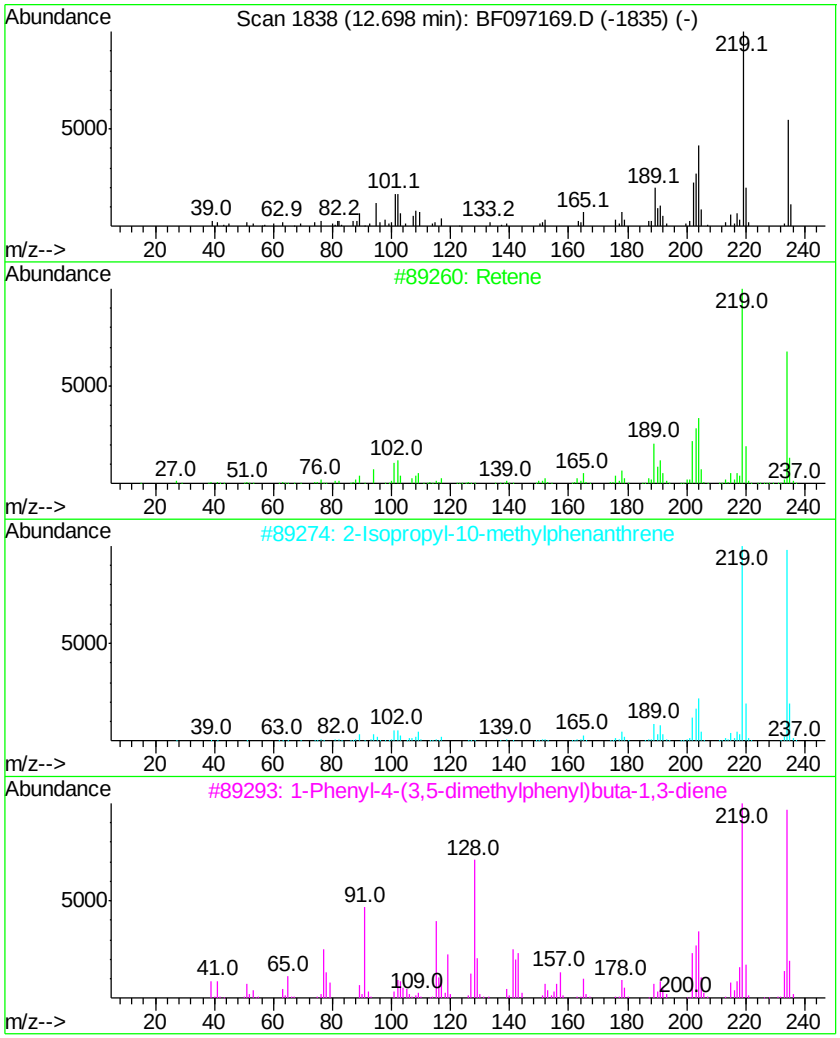
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

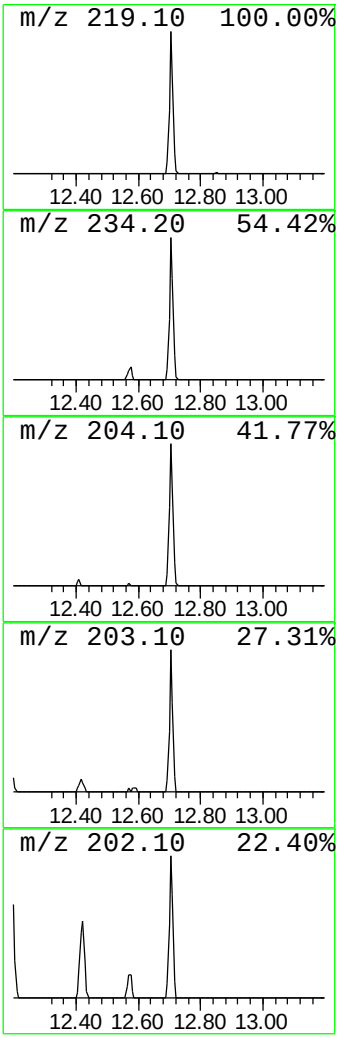
****

Peak Number 8 Retene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	6.19 ng	198456	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Retene	234	C18H18	000483-65-8	99
2	2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	98
3	1-Phenyl-4-(3,5-dimethylphenyl)b...	234	C18H18	1000202-15-0	83
4	Anthracene, 2-(1,1-dimethylethyl)-	234	C18H18	018801-00-8	81
5	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	50





Library Search Compound Report

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Data File : BF097169.D
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Sample : I4456-02
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Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

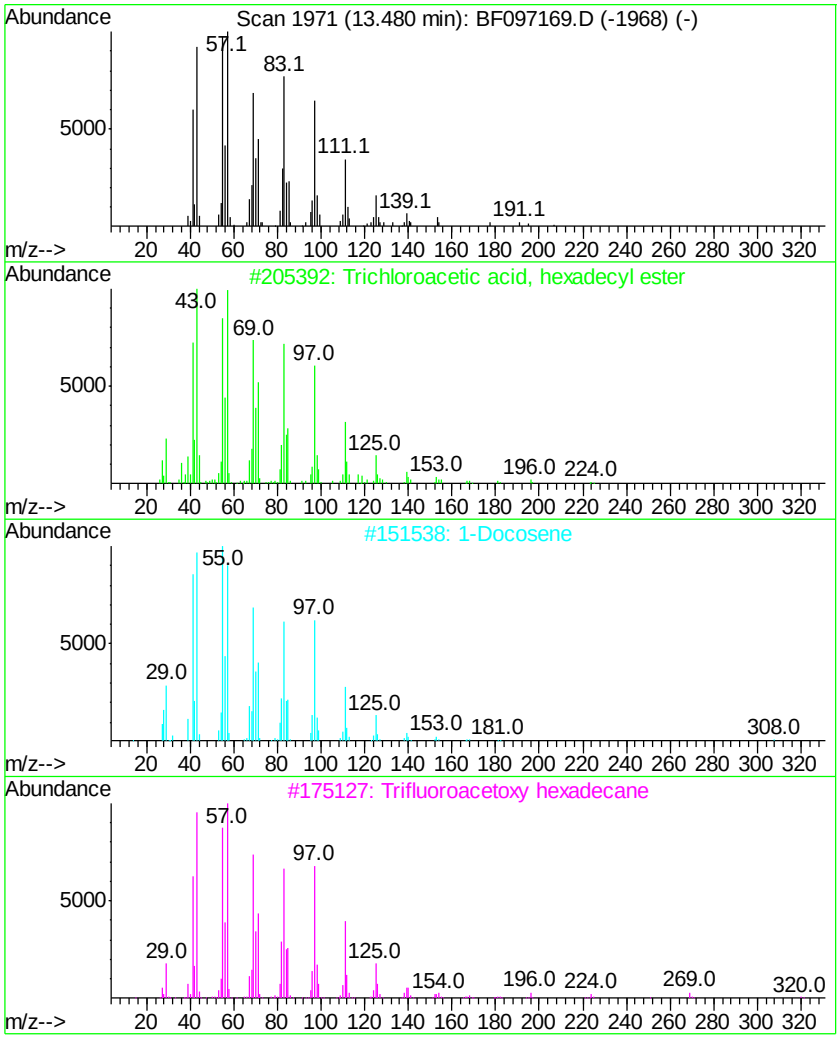
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

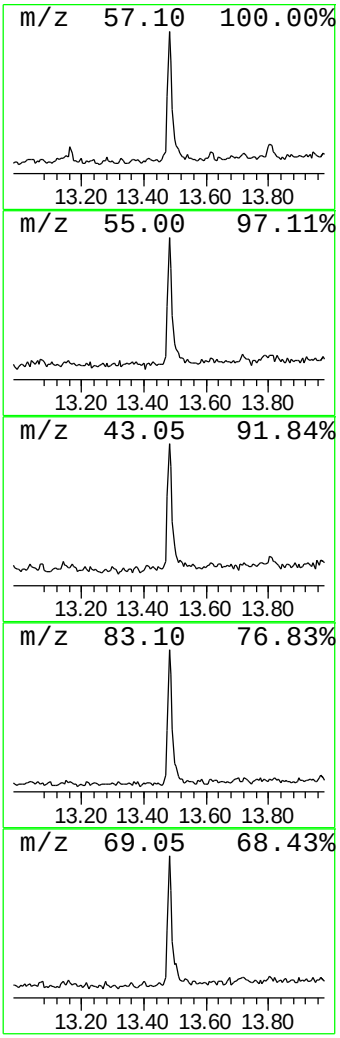
****

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	6.22 ng	199412	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097169.D
Acq On : 28 Jul 2017 22:22
Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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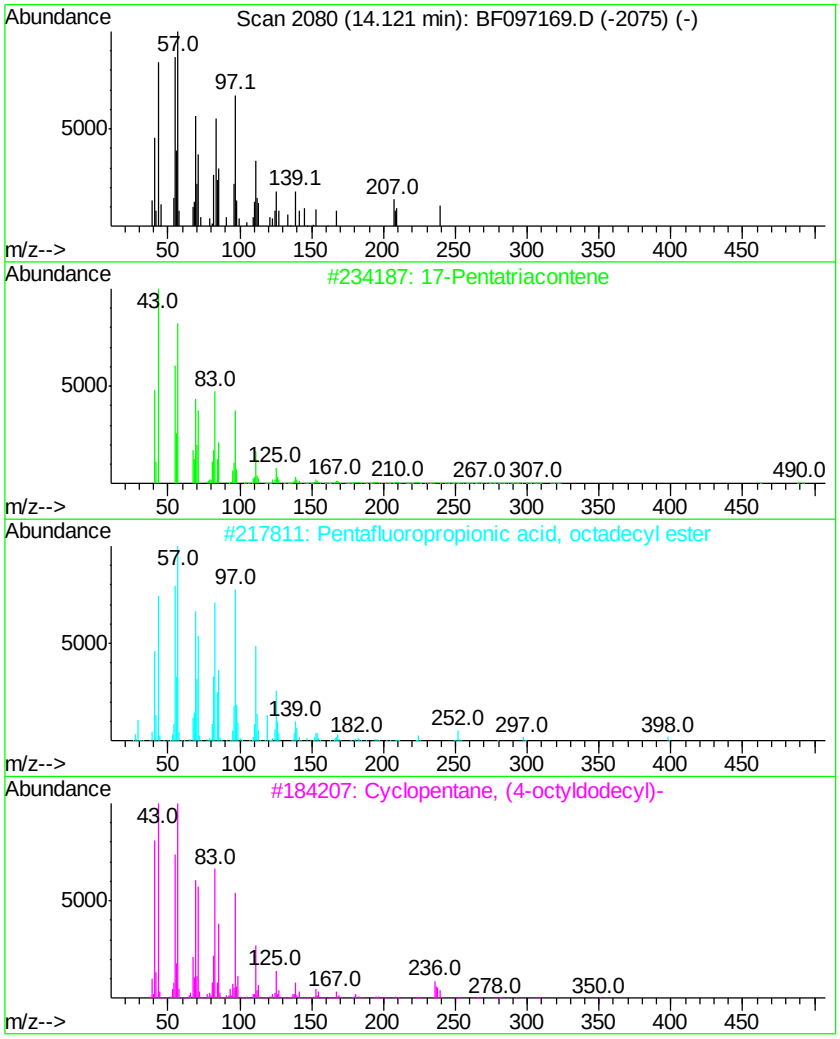
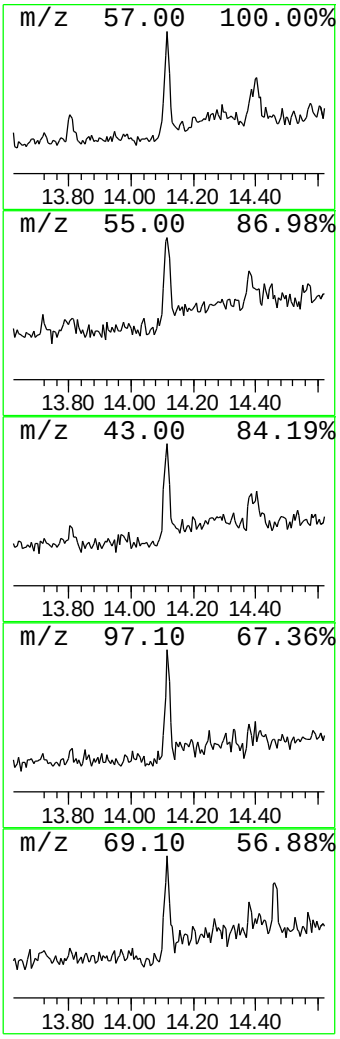
Peak Number 10 17-Pentatriacontene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.12	2.20 ng	70534	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	87
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	83
3	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	83
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	80
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	74





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097169.D
Acq On : 28 Jul 2017 22:22
Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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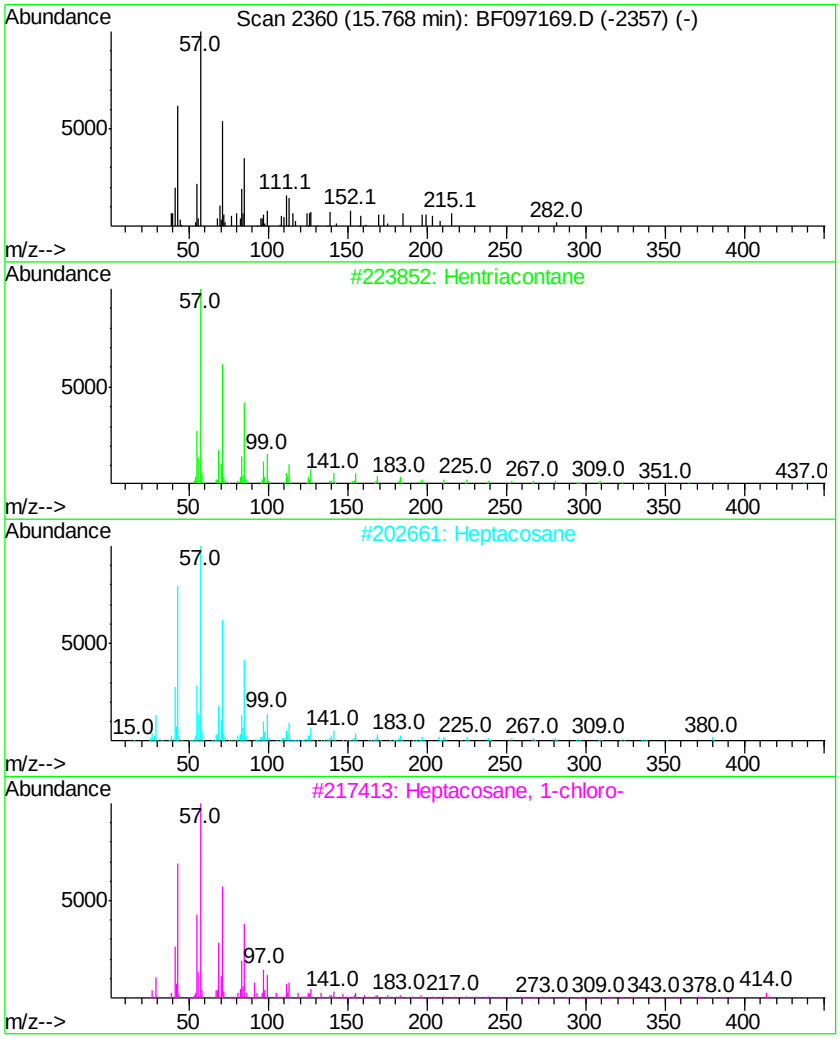
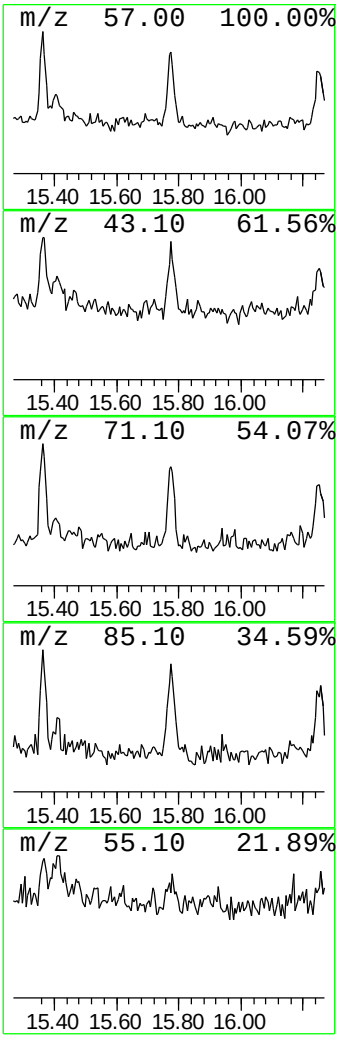
Peak Number 11 Hentriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.02 ng	51525	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	72
2	Heptacosane	380	C27H56	000593-49-7	64
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	59
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	58
5	Tritetracontane	605	C43H88	007098-21-7	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097169.D
Acq On : 28 Jul 2017 22:22
Operator : SJ/JU
Sample : I4456-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7D78

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	23.1	ng	867230	1	6.49	752546	20.0
unknown6.26	6.26	74.2	ng	2793260	1	6.49	752546	20.0
Hexadecane	10.44	2.6	ng	81598	4	10.99	616941	20.0
1-Hexadecanol	11.24	5.5	ng	171127	4	10.99	616941	20.0
3-Eicosyne	11.84	2.1	ng	65794	4	10.99	616941	20.0
5-Eicosene, (E)-	12.05	2.4	ng	75388	4	10.99	616941	20.0
Retene	12.70	6.2	ng	198456	5	13.61	640867	20.0
Trichloroacetic a...	13.48	6.2	ng	199412	5	13.61	640867	20.0
17-Pentatriacontene	14.12	2.2	ng	70534	5	13.61	640867	20.0
Hentriacontane	15.77	2.0	ng	51525	6	14.96	511334	20.0