LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116491.D
Acq On : 23 Aug 2019 21:39
Operator : HP/JU
Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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	2.187	11	17	23	rVB	2087164	2756012	100.00%	10.762%
2	5.499	575	580	583	rBV	2138081	1971195	71.52%	7.697%
3	6.504	745	751	754	rBV	1921346	1961046	71.16%	7.657%
4	6.651	771	776	779	rBV	2262135	2041657	74.08%	7.972%
5	6.881	812	815	819	rBV	727717	577723	20.96%	2.256%
6	7.040	838	842	845	rVB	1925259	1551689	56.30%	6.059%
7	7.122	853	856	861	rBV	31776	34524	1.25%	0.135%
8	7.204	865	870	873	rVB	41917	35565	1.29%	0.139%
9	7.440	904	910	913	rBV	1253952	1231186	44.67%	4.808%
10	7.651	941	946	948	rBV	67169	54055	1.96%	0.211%
11	7.681	948	951	957	rVB	130004	103389	3.75%	0.404%
12	7.904	986	989	992	rVB	55069	42475	1.54%	0.166%
13	8.163	1029	1033	1035	rBV	779724	660052	23.95%	2.577%
14	8.181	1035	1036	1041	rVB	73139	58753	2.13%	0.229%
15	8.910	1157	1160	1165	rVB	37984	38317	1.39%	0.150%
16	9.234	1211	1215	1218	rBV	2207591	1692257	61.40%	6.608%
17	9.622	1278	1281	1286	rBV	143186	115510	4.19%	0.451%
18	9.786	1303	1309	1311	rBV3	29907	38171	1.39%	0.149%
19	9.910	1325	1330	1334	rBV	753972	620306	22.51%	2.422%
20	10.292	1392	1395	1398	rBV5	20625	32699	1.19%	0.128%
21	10.328	1398	1401	1404	rVV2	59873	56390	2.05%	0.220%
22	10.381	1407	1410	1416	rVV5	36417	50677	1.84%	0.198%
23	10.457	1420	1423	1427	rVV	42158	40798	1.48%	0.159%
24	10.692	1459	1463	1467	rBV	1105137	914048	33.17%	3.569%
25	11.392	1579	1582	1584	rBV	584971	482706	17.51%	1.885%
26	11.416	1584	1586	1589	rVB	219264	165689	6.01%	0.647%
27	11.928	1670	1673	1675	rBV	250583	241554	8.76%	0.943%
28	12.527	1772	1775	1780	rBV	128798	145028	5.26%	0.566%
29	12.604	1785	1788	1791	rVV	441399	367045	13.32%	1.433%
30	12.833	1824	1827	1830	rVB	341344	286137	10.38%	1.117%
31	12.886	1833	1836	1838	rBV	324198	273257	9.91%	1.067%
32	12.980	1848	1852	1855	rBV	1352049	1248798	45.31%	4.876%
33	13.874	2001	2004	2014	rBV4	315957	454716	16.50%	1.776%
34	14.027	2026	2030	2033	rBV2	661084	812237	29.47%	3.172%

LSC Area Percent Report

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Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.563	2119	2121	2127	rVB	498032	563072	20.43%	2.199%
36	15.480	2275	2277	2279	rBV	328911	357314	12.96%	1.395%
37	15.668	2306	2309	2315	rVB3	401345	605964	21.99%	2.366%
38	16.245	2403	2407	2414	rVB	594980	1122382	40.72%	4.383%
39	16.686	2477	2482	2493	rVB	980777	1805091	65.50%	7.049%

Sum of corrected areas: 25609484

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
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Sample : K4385-19
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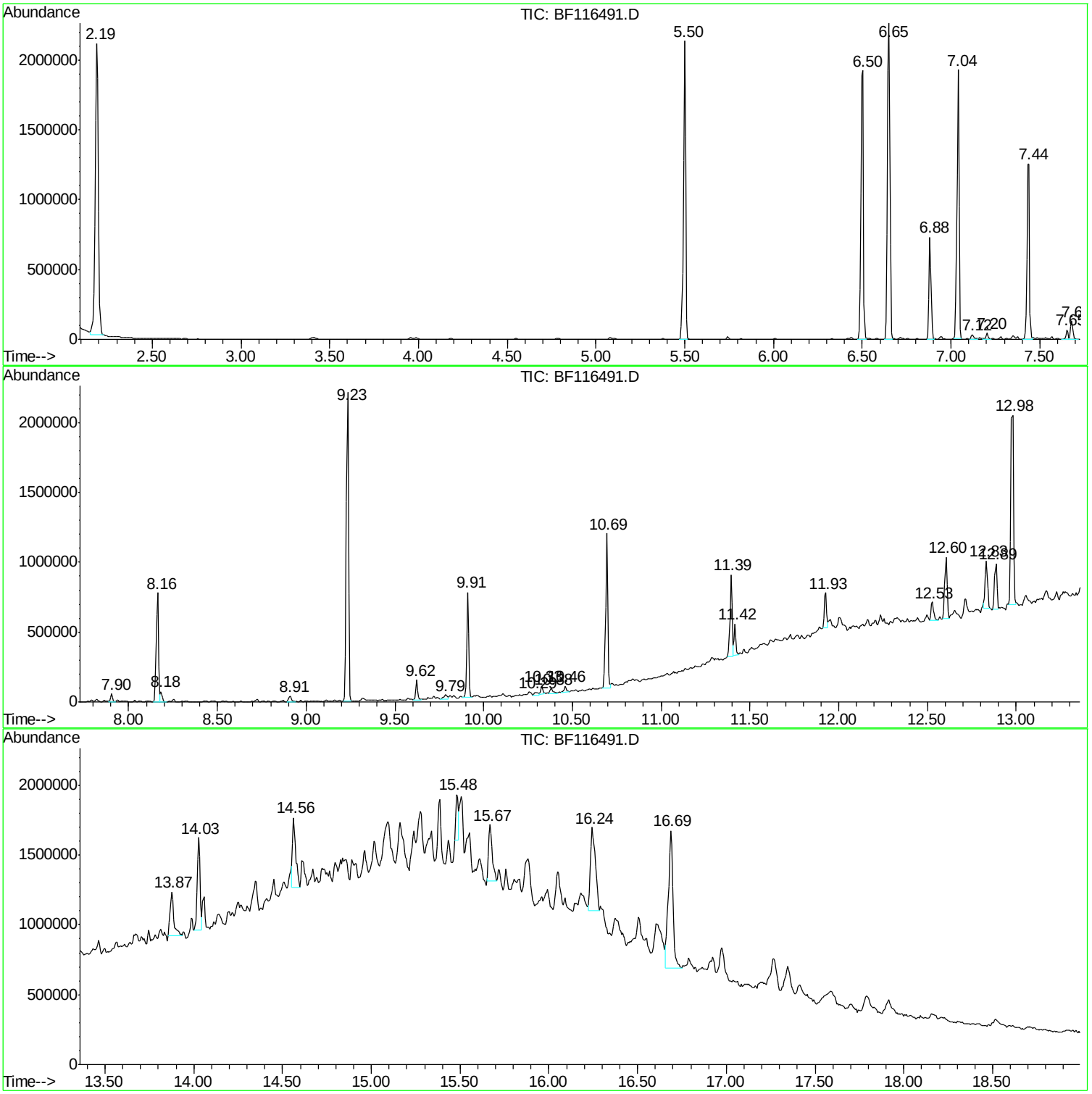
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116491.D
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Operator : HP/JU
Sample : K4385-19
Misc :
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Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

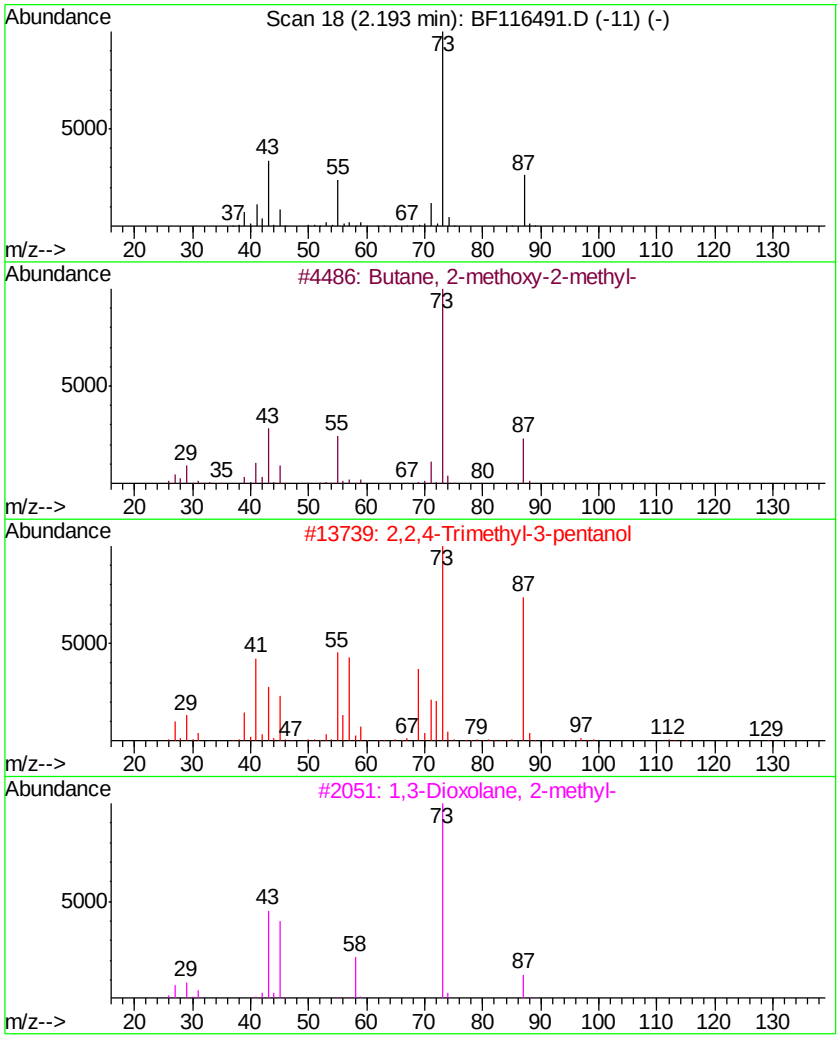
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

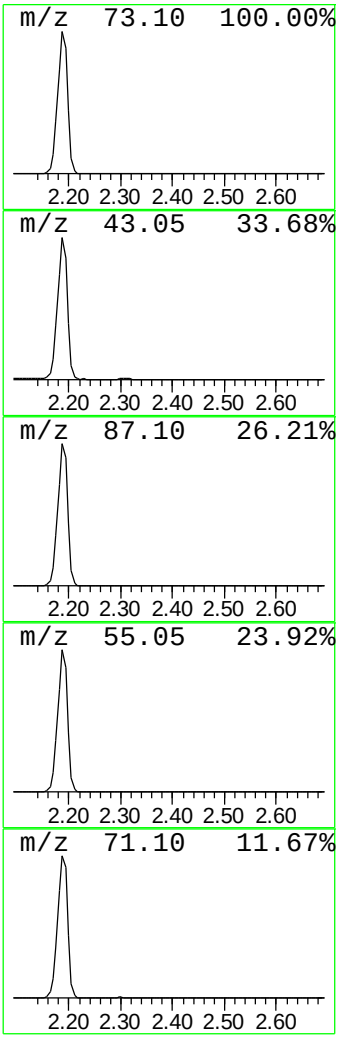
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	95.41 ng	2756010	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
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	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116491.D
Acq On : 23 Aug 2019 21:39
Operator : HP/JU
Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

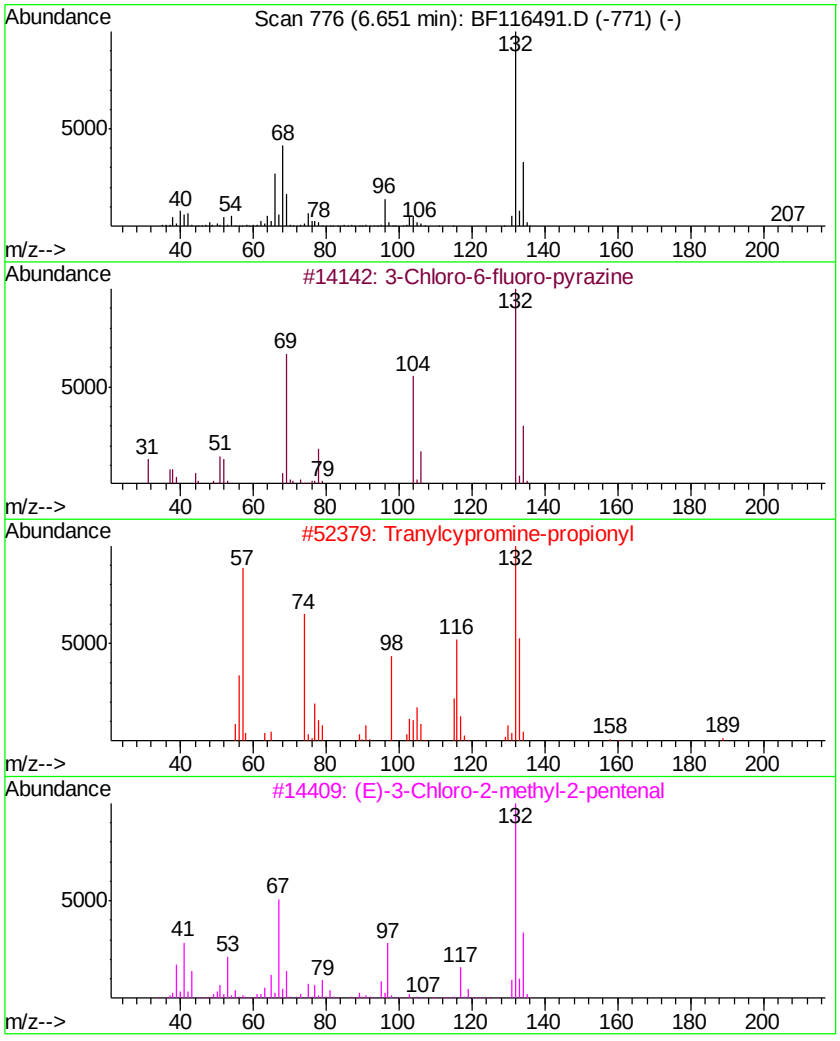
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

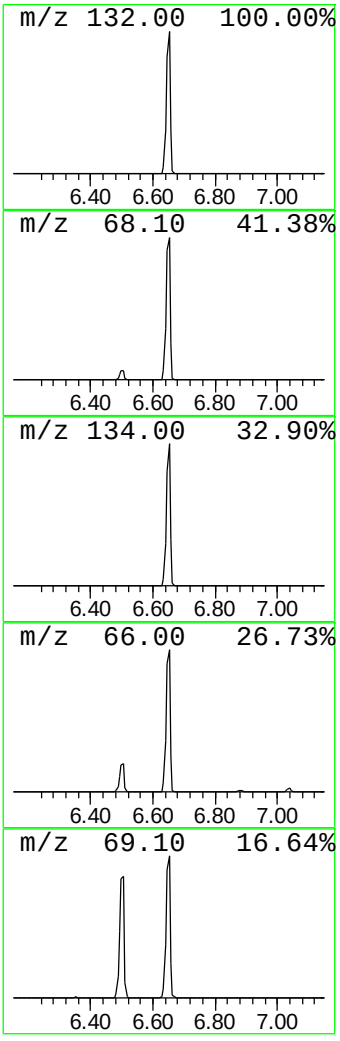
****

Peak Number 2 unknown6.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	70.68 ng	2041660	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116491.D
Acq On : 23 Aug 2019 21:39
Operator : HP/JU
Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

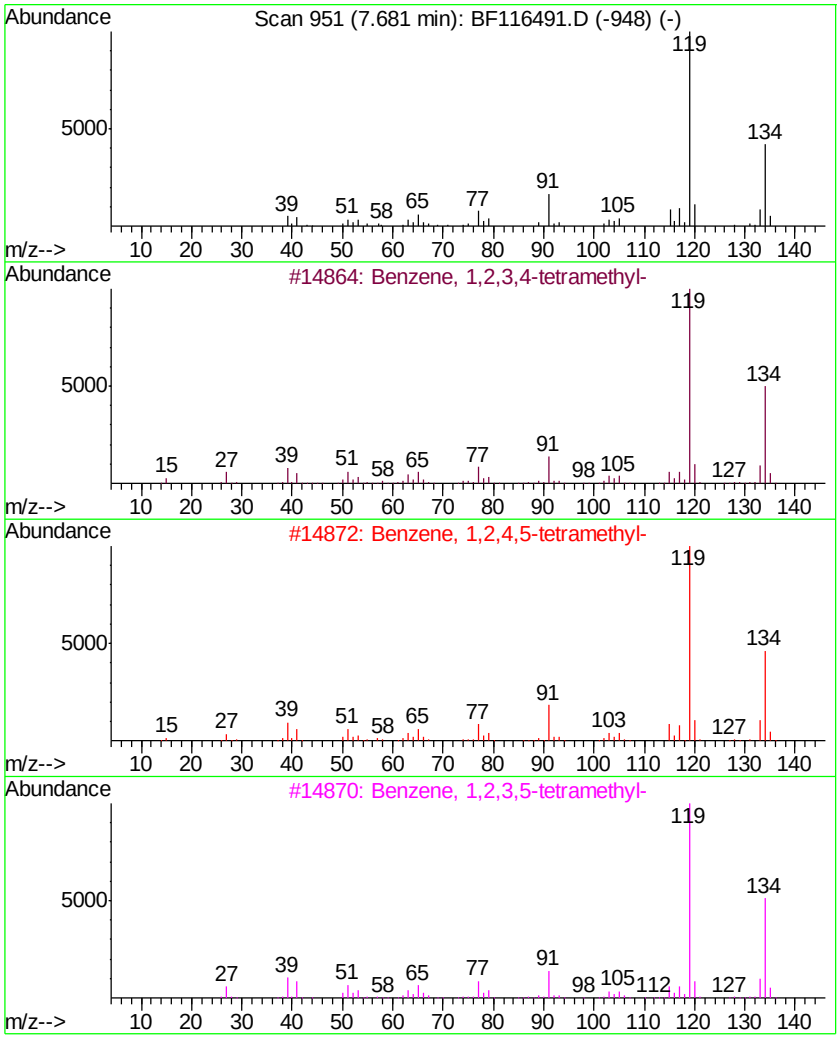
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

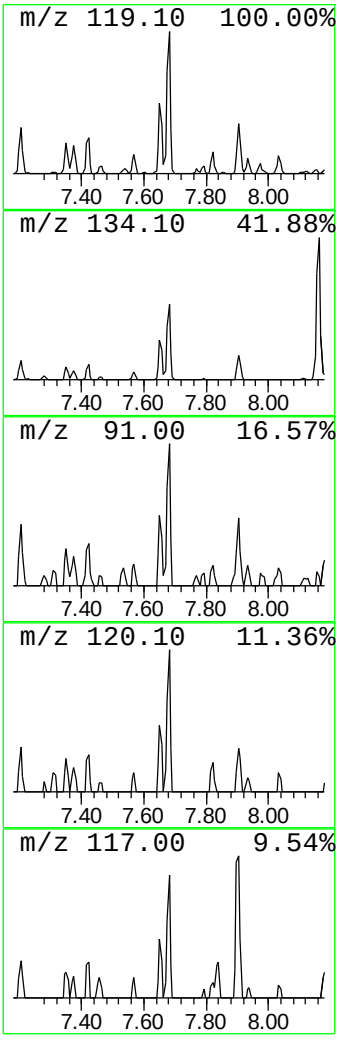
****

Peak Number 4 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	3.13 ng	103389	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	p-Cymene	134	C10H14	000099-87-6	94





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116491.D
Acq On : 23 Aug 2019 21:39
Operator : HP/JU
Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

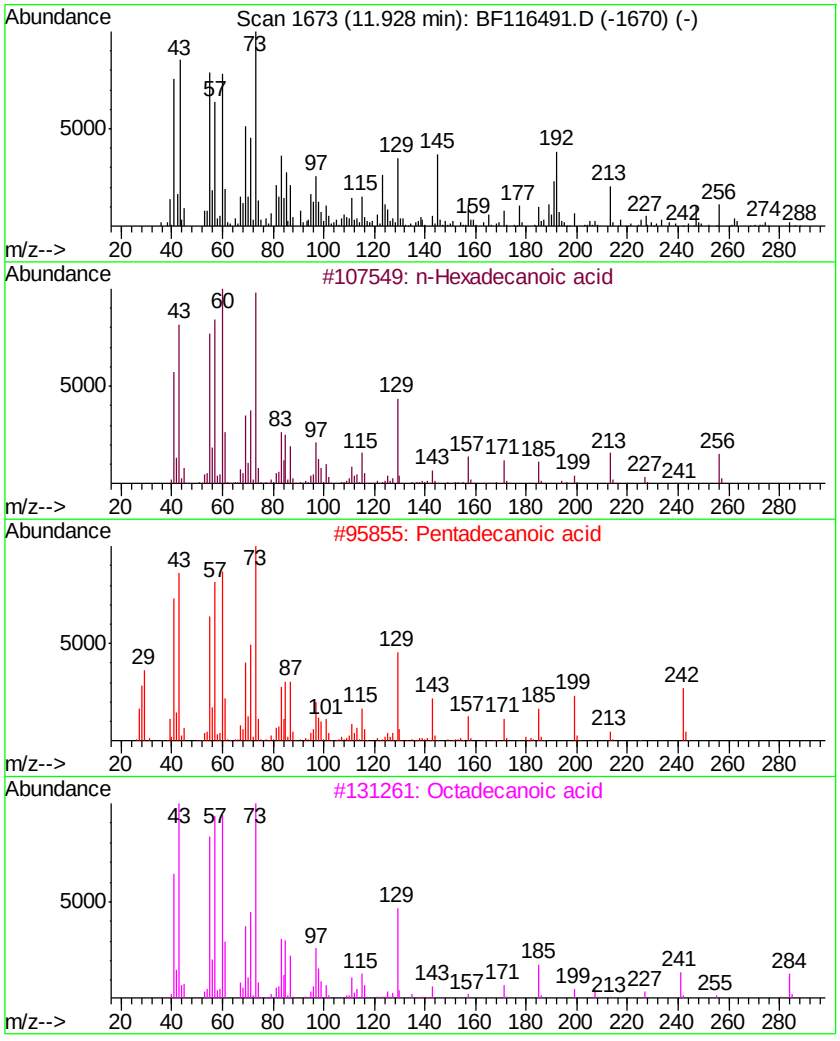
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

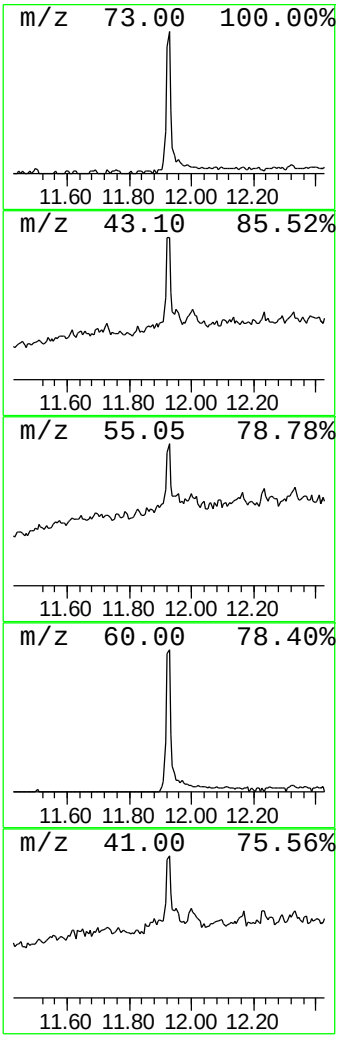
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	10.01 ng	241554	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	41
3	Octadecanoic acid	284	C18H36O2	000057-11-4	38
4	N-Cyclododecylacetamide	225	C14H27NO	026093-81-2	35
5	Dodecanoic acid	200	C12H24O2	000143-07-7	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
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Acq On : 23 Aug 2019 21:39
Operator : HP/JU
Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

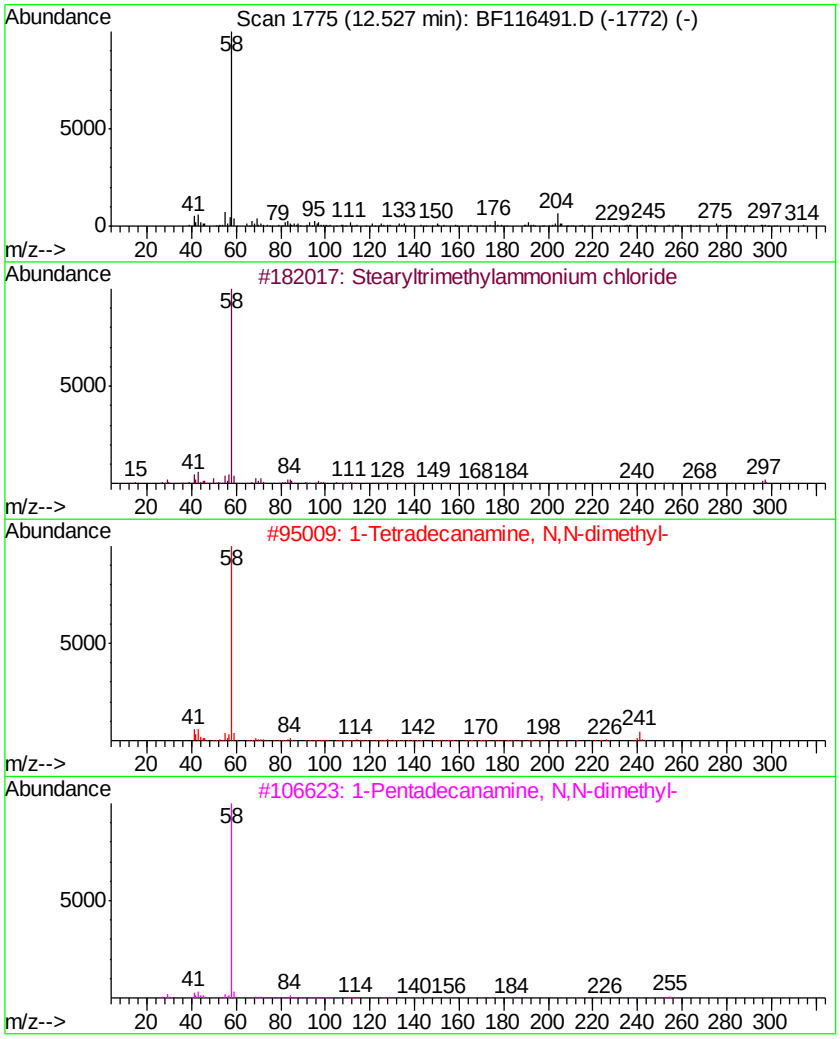
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

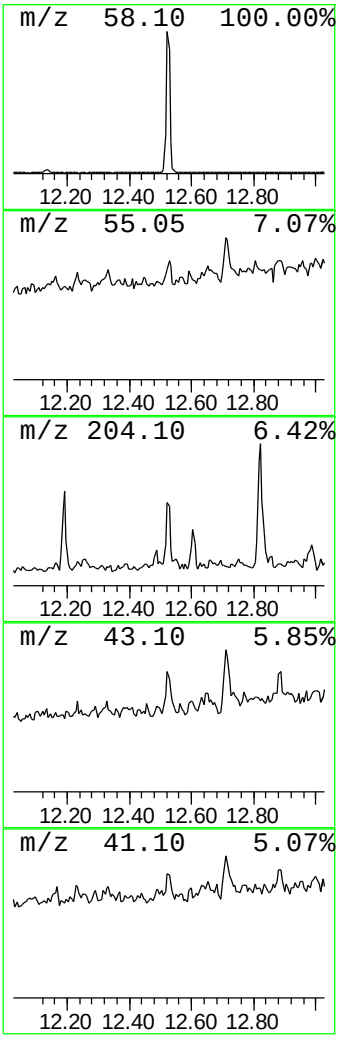
****

Peak Number 6 Stearyltrimethylammonium ch... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	6.01 ng	145028	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stearyltrimethylammonium chloride	347	C21H46ClN	000112-03-8	72
2	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	64
3	1-Pentadecanamine, N,N-dimethyl-	255	C17H37N	017678-60-3	64
4	Dimethyl palmitamine	269	C18H39N	000112-69-6	64
5	1-Heptadecanamine, N,N-dimethyl-	283	C19H41N	003002-57-1	64





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Acq On : 23 Aug 2019 21:39
Operator : HP/JU
Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

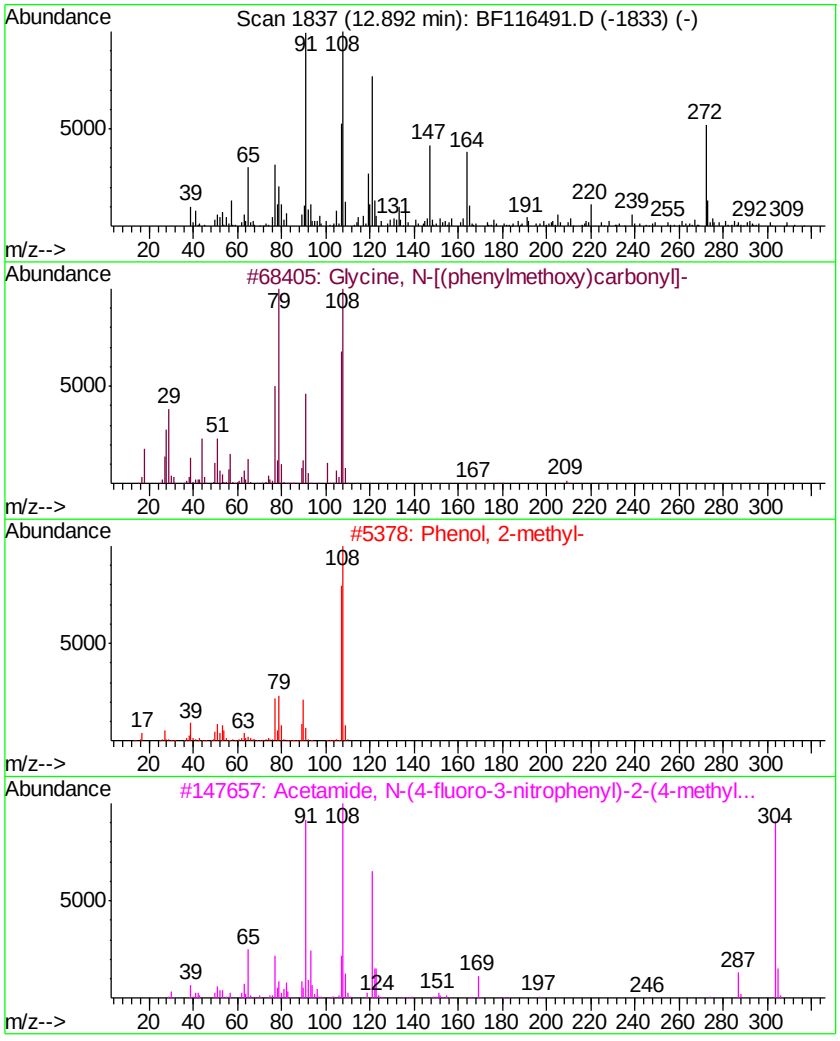
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

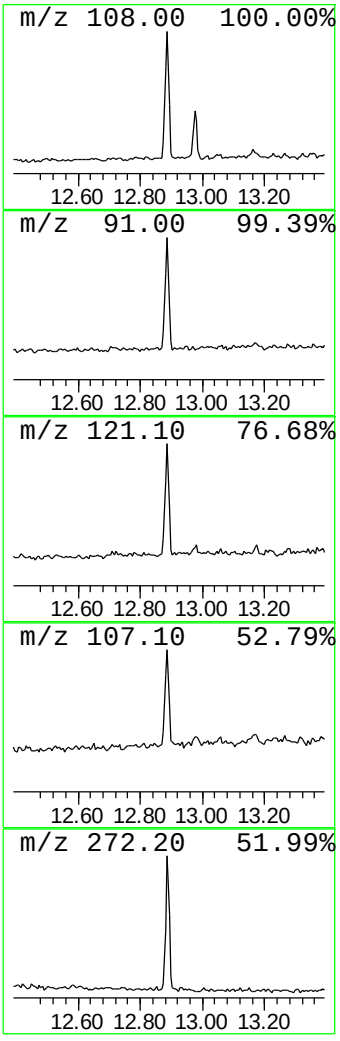
****

Peak Number 7 Glycine, N-[(phenylmethoxy)... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	6.73 ng	273257	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycine, N-[(phenylmethoxy)carbo...	209	C10H11NO4	001138-80-3	50
2	Phenol, 2-methyl-	108	C7H8O	000095-48-7	43
3	Acetamide, N-(4-fluoro-3-nitroph...	304	C15H13FN2O4	1000317-28-8	41
4	Oxalic acid, ethyl 2-methylpheny...	208	C11H12O4	1000309-59-1	38
5	Ethanol, 2-(4-methylphenoxy)-	152	C9H12O2	015149-10-7	38





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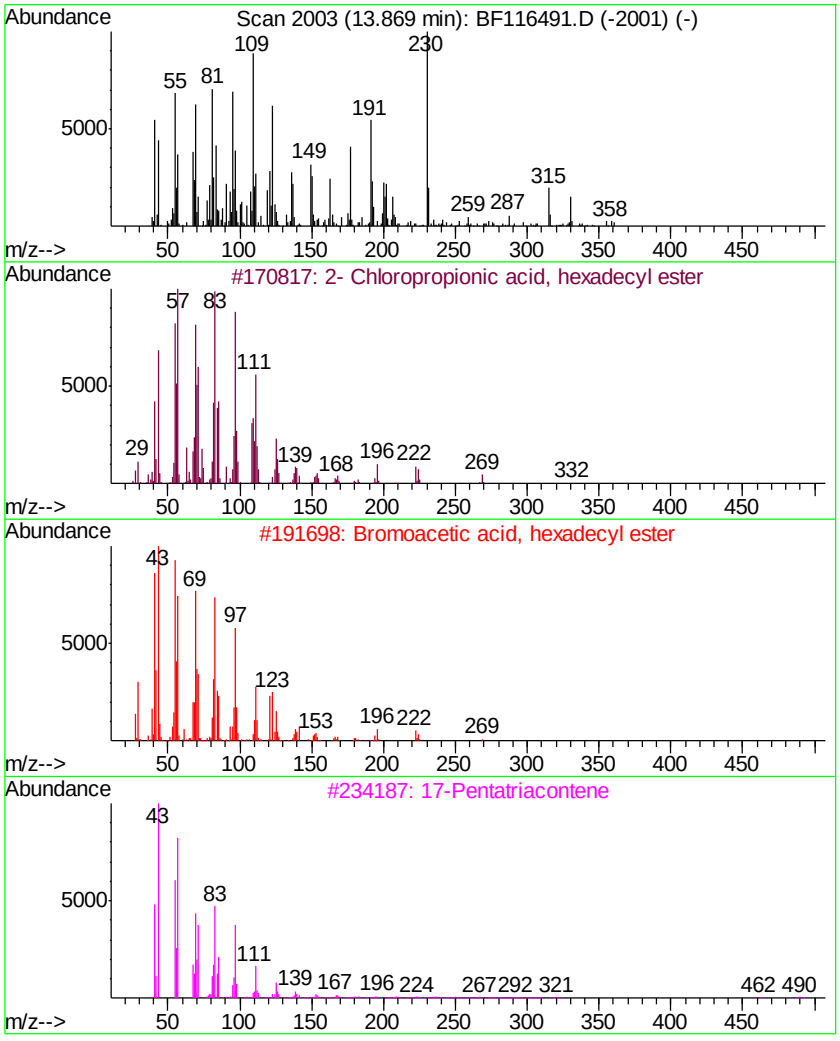
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

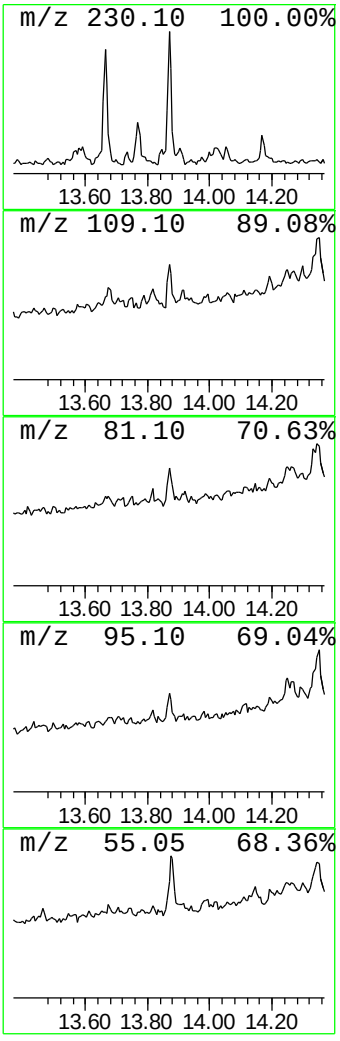
****

Peak Number 8 2- Chloropropionic acid, he... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	11.20 ng	454716	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	56
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	55
3	17-Pentatriacontene	491	C35H70	006971-40-0	50
4	Disparlure	282	C19H38O	029804-22-6	47
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	46





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Data File : BF116491.D
Acq On : 23 Aug 2019 21:39
Operator : HP/JU
Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

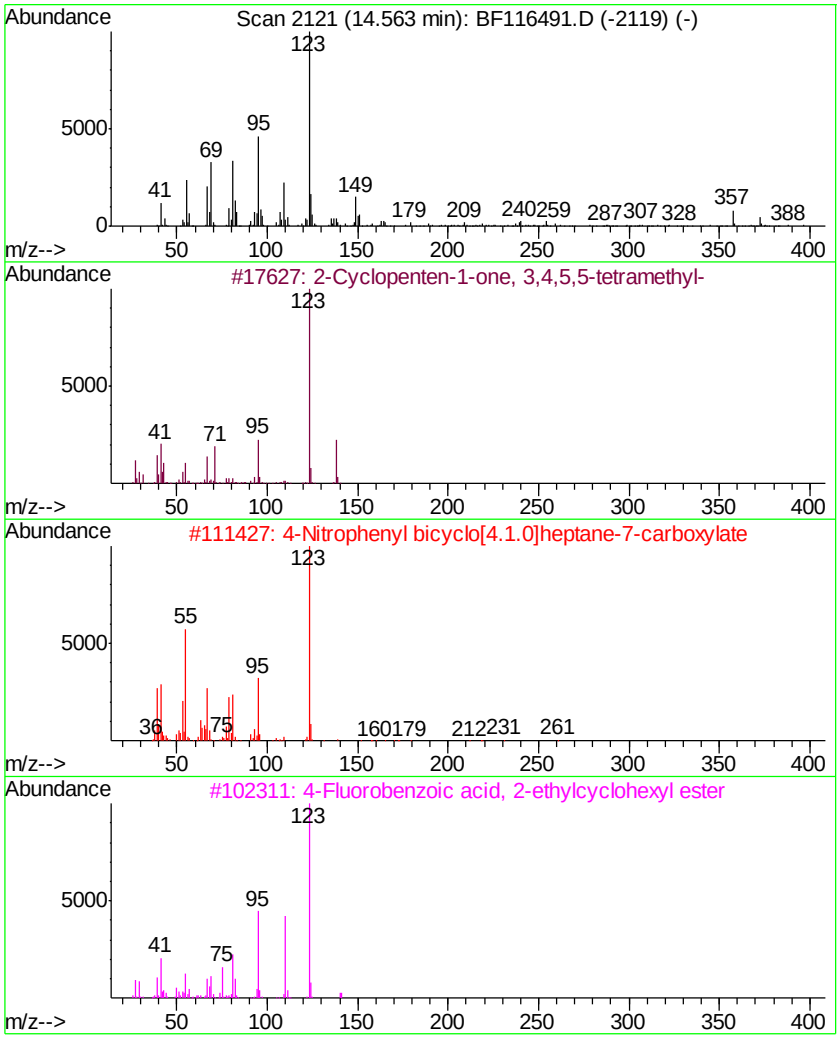
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

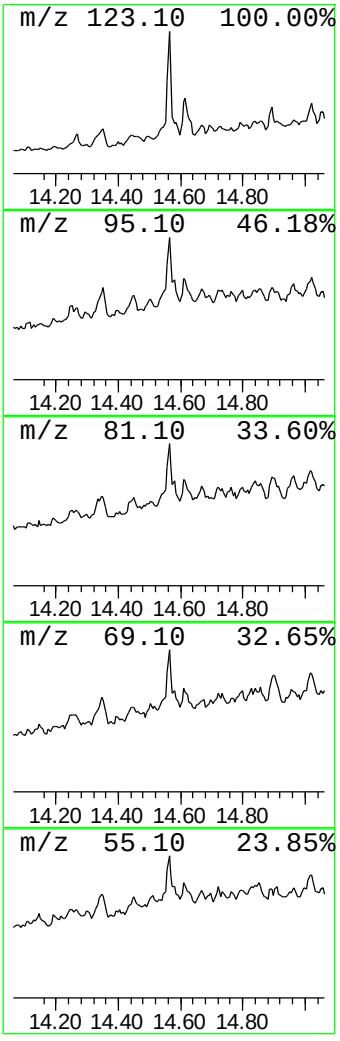
****

Peak Number 9 2-Cyclopenten-1-one, 3,4,5,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	13.86 ng	563072	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 3,4,5,5-tet...	138	C9H14O	090611-02-2	59
2	4-Nitrophenyl bicyclo[4.1.0]hept...	261	C14H15NO4	328938-65-4	59
3	4-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-06-0	53
4	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	53
5	4-Fluoro-N-(1H-tetrazol-5-yl)ben...	207	C8H6FN5O	1000306-76-6	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116491.D
Acq On : 23 Aug 2019 21:39
Operator : HP/JU
Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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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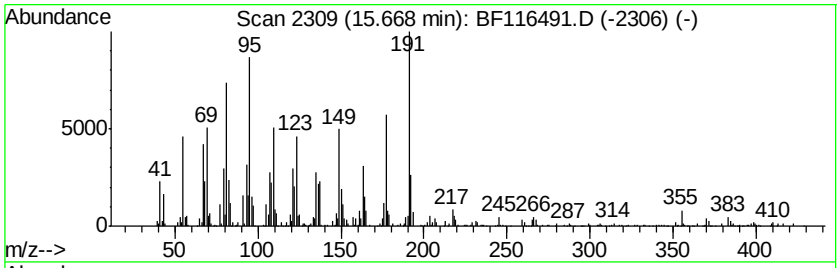
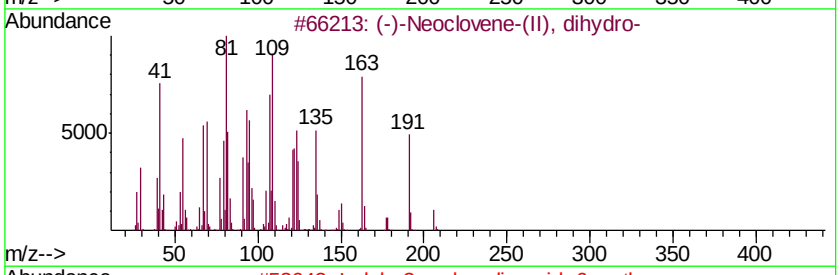
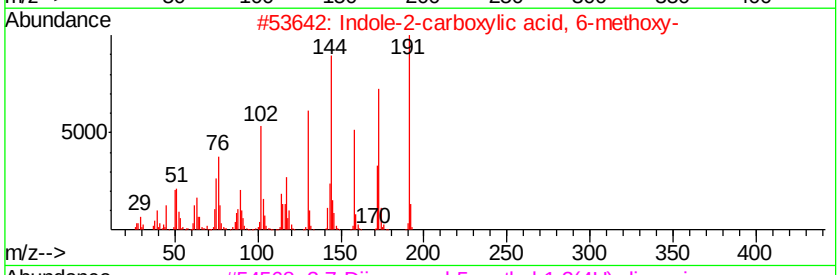
Peak Number 10 unknown15.67 Concentration Rank 6

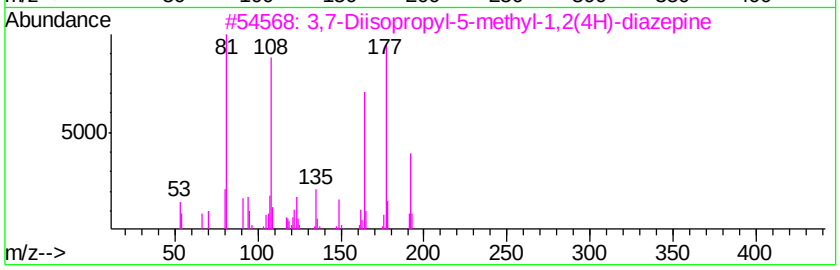
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	33.92 ng	605964	Perylene-d12	15.50

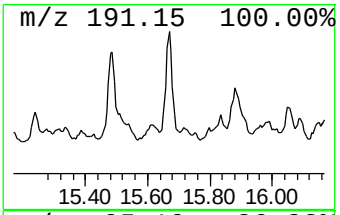
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	44
2	Indole-2-carboxylic acid, 6-meth...	191	C10H9NO3	016732-73-3	25
3	3,7-Diisopropyl-5-methyl-1,2(4H)...	192	C12H20N2	088829-71-4	22
4	Squalene	410	C30H50	000111-02-4	18
5	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	14

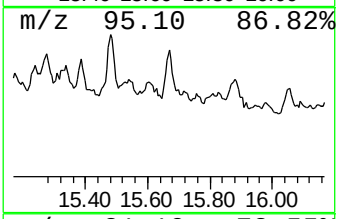


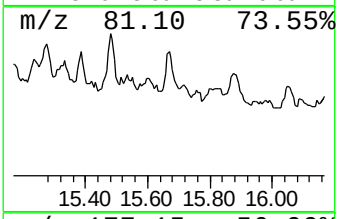


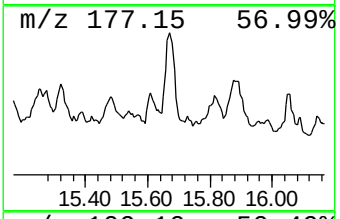


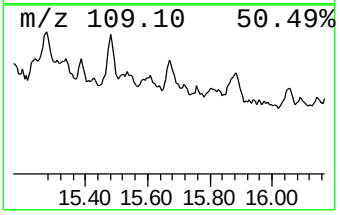












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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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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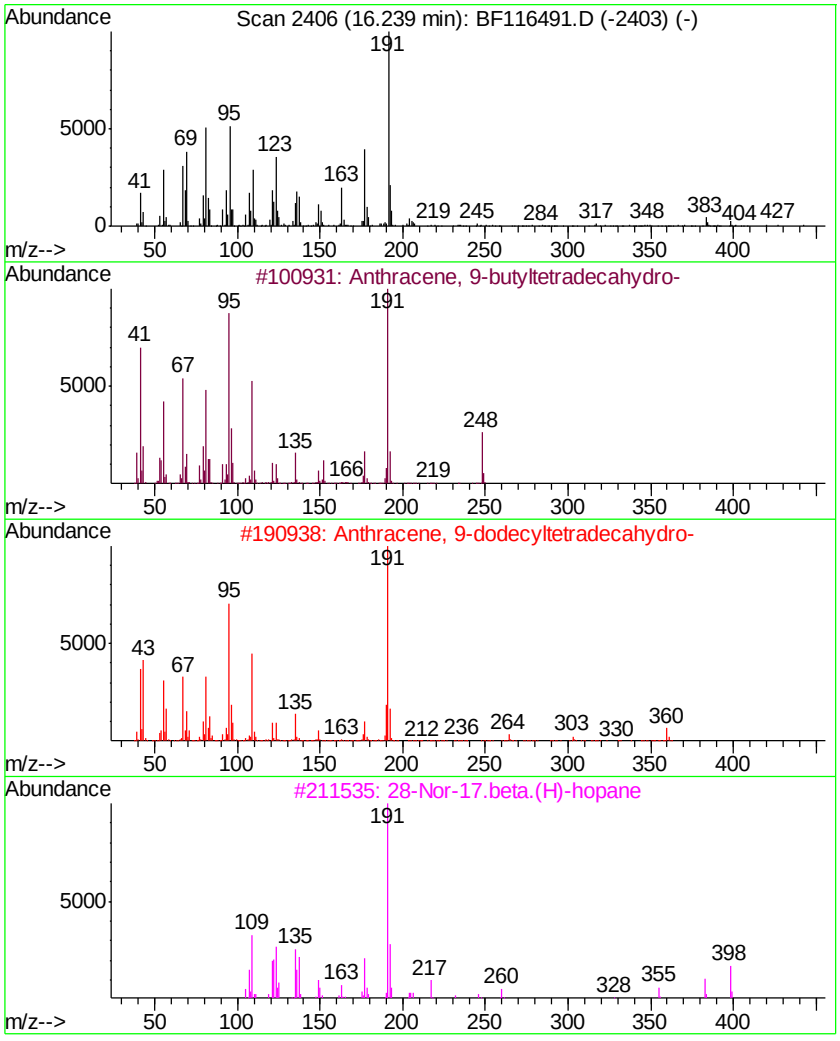
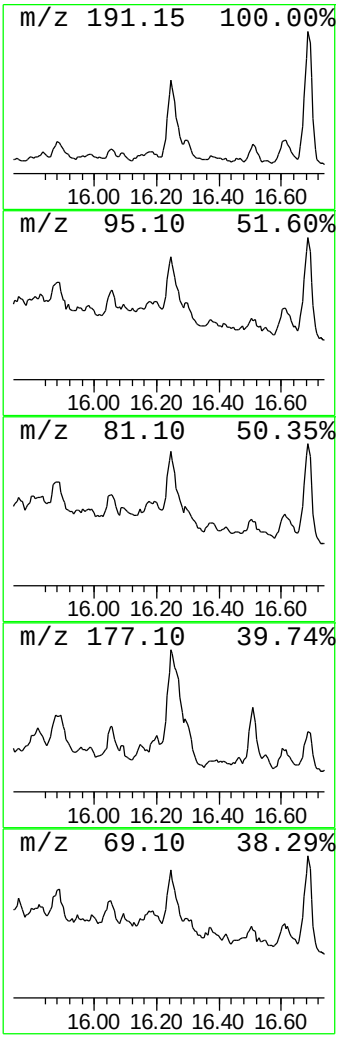
Peak Number 11 unknown16.24 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	62.82 ng	1122380	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	40
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	38
3	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	32
4	4-Fluoro-2-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-67-0	27
5	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	25





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Sample : K4385-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T8-E1-E4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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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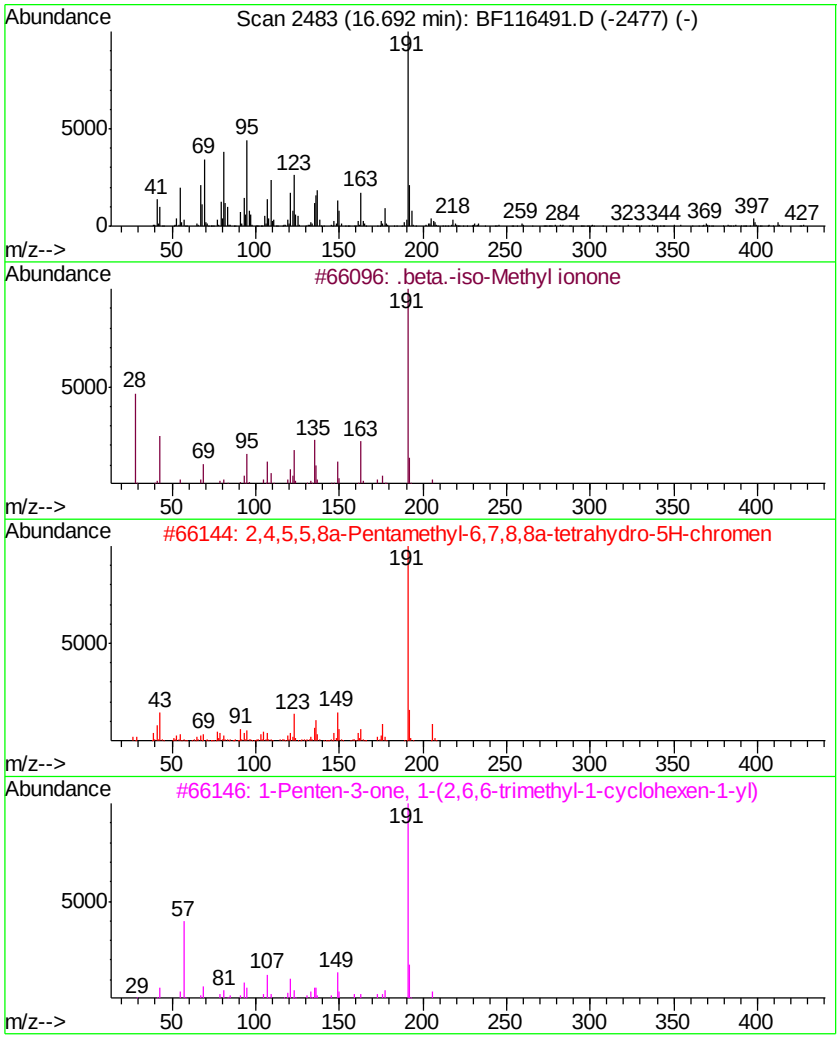
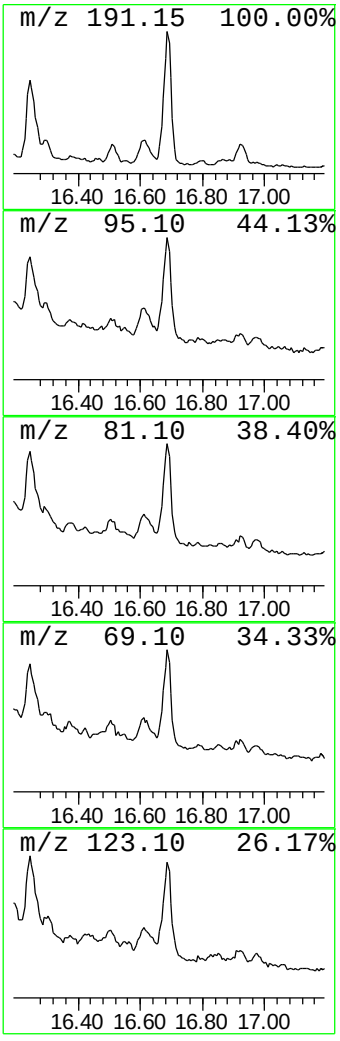
Peak Number 12 .beta.-iso-Methyl ionone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	101.04 ng	1805090	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	72
2	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	47
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	45
4	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	38
5	4-(3H-Imidazo[4,5-b]pyridin-2-yl...	342	C15H18N8S	1000276-08-2	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082319\
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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...	2.19	95.4	ng	2756010	1	6.88	577723	20.0
unknown6.65	6.65	70.7	ng	2041660	1	6.88	577723	20.0
Benzene, 1,2,3,4-...	7.68	3.1	ng	103389	2	8.16	660052	20.0
n-Hexadecanoic acid	11.93	10.0	ng	241554	4	11.39	482706	20.0
Stearyltrimethyla...	12.53	6.0	ng	145028	4	11.39	482706	20.0
Glycine, N-[(phen...	12.89	6.7	ng	273257	5	14.03	812237	20.0
2- Chloropropioni...	13.87	11.2	ng	454716	5	14.03	812237	20.0
2-Cyclopenten-1-o...	14.56	13.9	ng	563072	5	14.03	812237	20.0
unknown15.67	15.67	33.9	ng	605964	6	15.50	357314	20.0
unknown16.24	16.24	62.8	ng	1122380	6	15.50	357314	20.0
.beta.-iso-Methyl...	16.69	101.0	ng	1805090	6	15.50	357314	20.0