LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103462.D
Acq On : 6 Mar 2018 18:23
Operator : SJ/JU
Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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-BF022218.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	195782	263917	7.46%	0.732%
2	5.110	511	514	530	rBV	56554	98246	2.78%	0.273%
3	5.498	576	580	612	rBV	2492711	3539741	100.00%	9.818%
4	6.510	748	752	771	rBV	2524175	3435721	97.06%	9.530%
5	6.645	771	775	786	rVV	2913467	3245265	91.68%	9.001%
6	6.869	809	813	835	rVB	890885	972649	27.48%	2.698%
7	7.022	835	839	858	rBV	2227143	2493172	70.43%	6.915%
8	7.439	905	910	934	rBV	1831480	2354260	66.51%	6.530%
9	8.151	1028	1031	1051	rBV	1017032	1320206	37.30%	3.662%
10	9.027	1176	1180	1182	rBV	59137	53374	1.51%	0.148%
11	9.092	1187	1191	1200	rVB	246823	258129	7.29%	0.716%
12	9.227	1207	1214	1224	rBV	3090510	3348790	94.61%	9.289%
13	9.333	1229	1232	1237	rVV2	33367	40863	1.15%	0.113%
14	9.404	1240	1244	1255	rVB3	26772	55672	1.57%	0.154%
15	9.704	1292	1295	1304	rVB2	42918	51085	1.44%	0.142%
16	9.910	1326	1330	1341	rVB	1305409	1287546	36.37%	3.571%
17	10.116	1361	1365	1374	rBV6	20086	47887	1.35%	0.133%
18	10.298	1393	1396	1398	rBV	106302	88725	2.51%	0.246%
19	10.322	1398	1400	1403	rVB	69275	54474	1.54%	0.151%
20	10.527	1431	1435	1442	rBV	171980	164434	4.65%	0.456%
21	10.710	1462	1466	1478	rBV	1511927	1783747	50.39%	4.948%
22	10.798	1478	1481	1485	rVB2	41956	53772	1.52%	0.149%
23	10.904	1494	1499	1503	rBV	48843	52085	1.47%	0.144%
24	11.063	1522	1526	1534	rBV6	20335	42097	1.19%	0.117%
25	11.245	1554	1557	1560	rBV	39565	36477	1.03%	0.101%
26	11.339	1570	1573	1576	rBV2	40836	35852	1.01%	0.099%
27	11.404	1581	1584	1587	rBV	1126193	1132206	31.99%	3.140%
28	11.427	1587	1588	1593	rVB2	185257	184531	5.21%	0.512%
29	11.551	1606	1609	1613	rVB	199505	160653	4.54%	0.446%
30	11.610	1615	1619	1624	rBV7	30868	42896	1.21%	0.119%
31	11.674	1624	1630	1632	rBV2	62312	63596	1.80%	0.176%
32	11.774	1644	1647	1651	rVB	42631	41562	1.17%	0.115%
33	11.927	1667	1673	1675	rBV	1496220	1619392	45.75%	4.492%
34	11.951	1675	1677	1683	rVB	797730	687209	19.41%	1.906%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103462.D
Acq On : 6 Mar 2018 18:23
Operator : SJ/JU
Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.080	1697	1699	1702	rBV	54972	43536	1.23%	0.121%
36	12.233	1722	1725	1732	rVB2	71355	84067	2.37%	0.233%
37	12.468	1762	1765	1768	rVV2	73762	65113	1.84%	0.181%
38	12.568	1778	1782	1787	rVB3	59475	81793	2.31%	0.227%
39	12.627	1787	1792	1800	rBV	336449	433663	12.25%	1.203%
40	12.710	1801	1806	1817	rBV	1023378	1181946	33.39%	3.278%
41	12.845	1825	1829	1830	rBV	161111	170643	4.82%	0.473%
42	12.857	1830	1831	1837	rVB	197155	166638	4.71%	0.462%
43	12.992	1849	1854	1857	rBV	2214395	2096520	59.23%	5.815%
44	13.198	1884	1889	1893	rVB2	197337	212144	5.99%	0.588%
45	13.539	1944	1947	1954	rBV	160782	156806	4.43%	0.435%
46	13.868	2000	2003	2008	rBV	326110	339421	9.59%	0.941%
47	14.010	2024	2027	2030	rBV	78272	66742	1.89%	0.185%
48	14.062	2031	2036	2039	rBV	818075	900230	25.43%	2.497%
49	14.192	2055	2058	2062	rVB	66510	60332	1.70%	0.167%
50	14.498	2108	2110	2118	rBV6	40758	59892	1.69%	0.166%
51	15.133	2214	2218	2220	rBV	78128	119242	3.37%	0.331%
52	15.574	2289	2293	2303	rVB	467732	703958	19.89%	1.953%

Sum of corrected areas: 36052917

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
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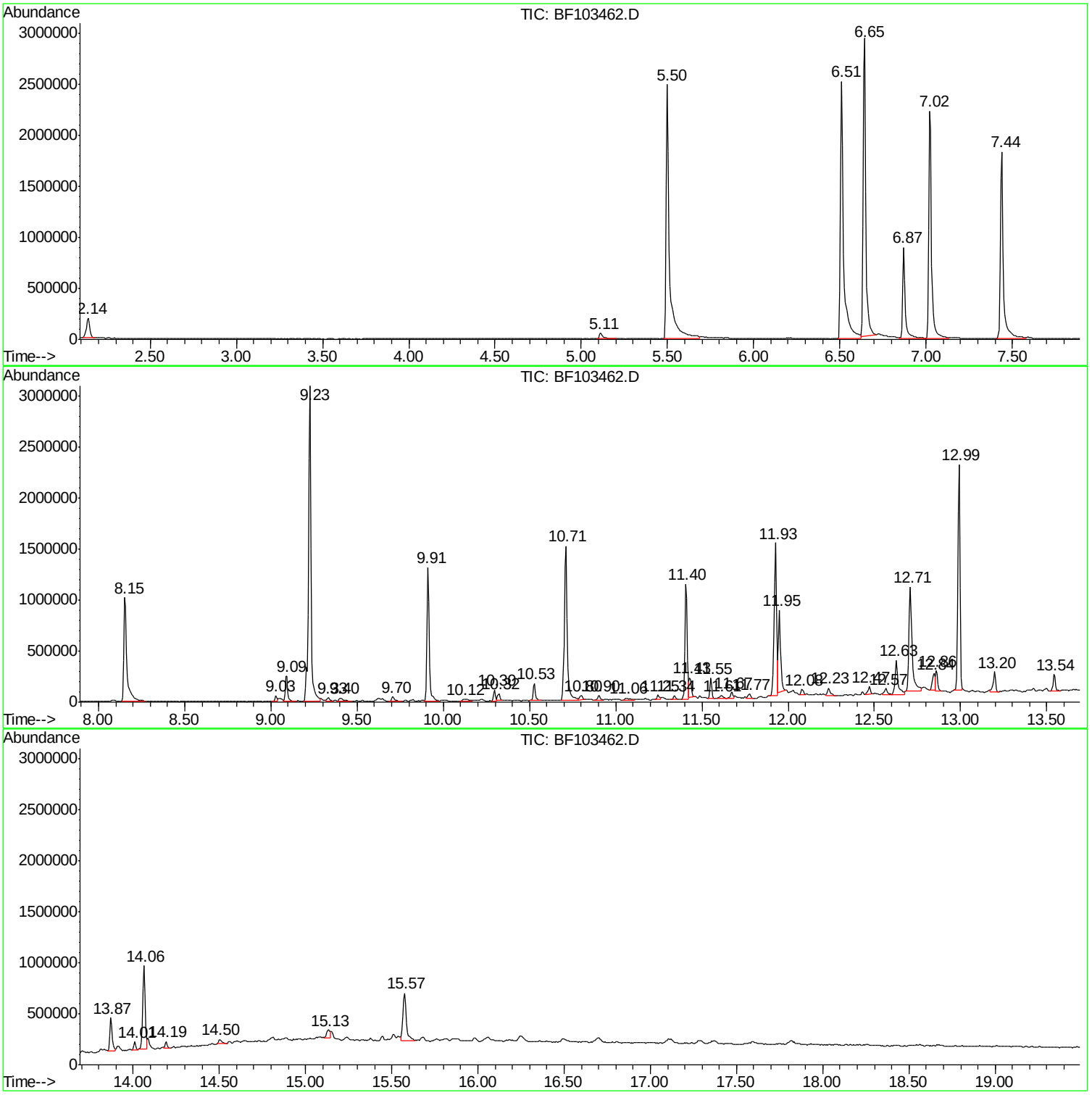
Operator : SJ/JU
Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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Data File : BF103462.D
Acq On : 6 Mar 2018 18:23
Operator : SJ/JU
Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

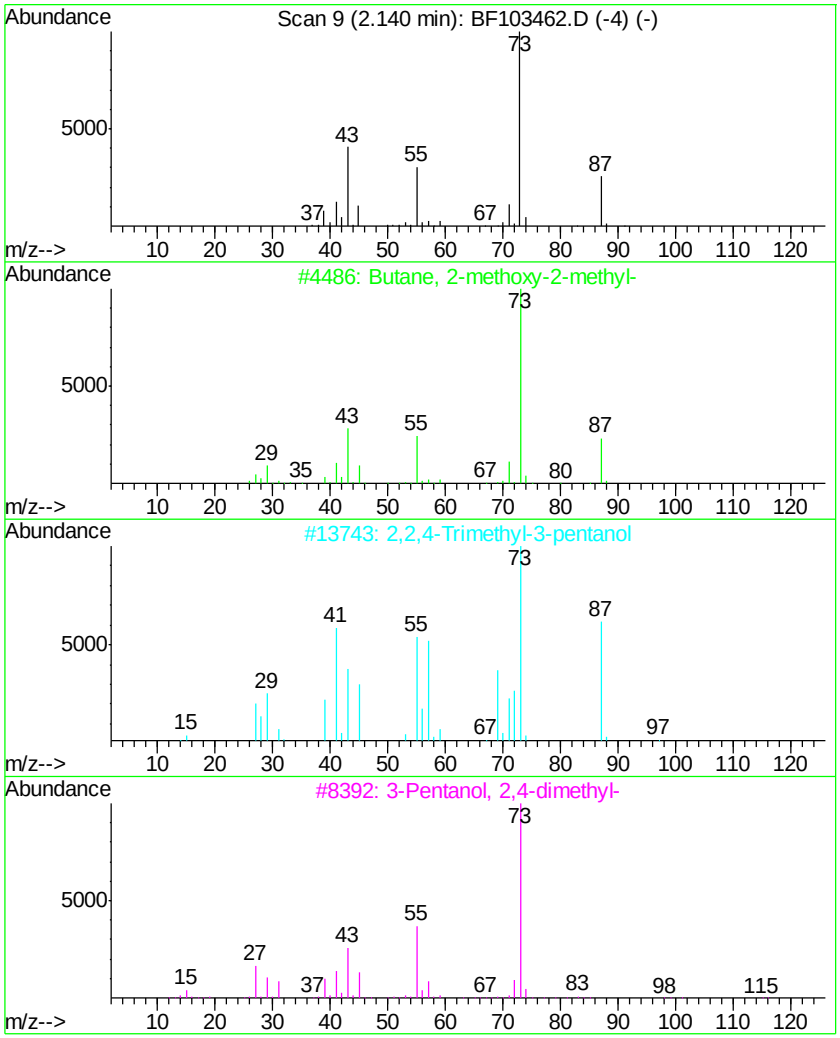
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

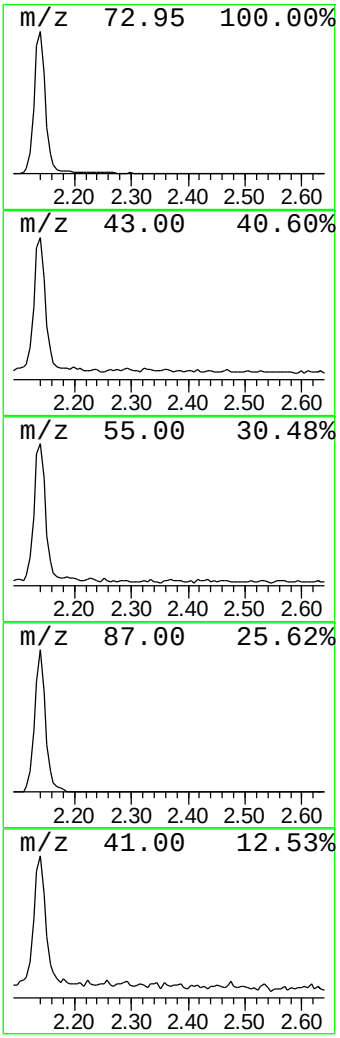
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	5.43 ng	263917	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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF103462.D
Acq On : 6 Mar 2018 18:23
Operator : SJ/JU
Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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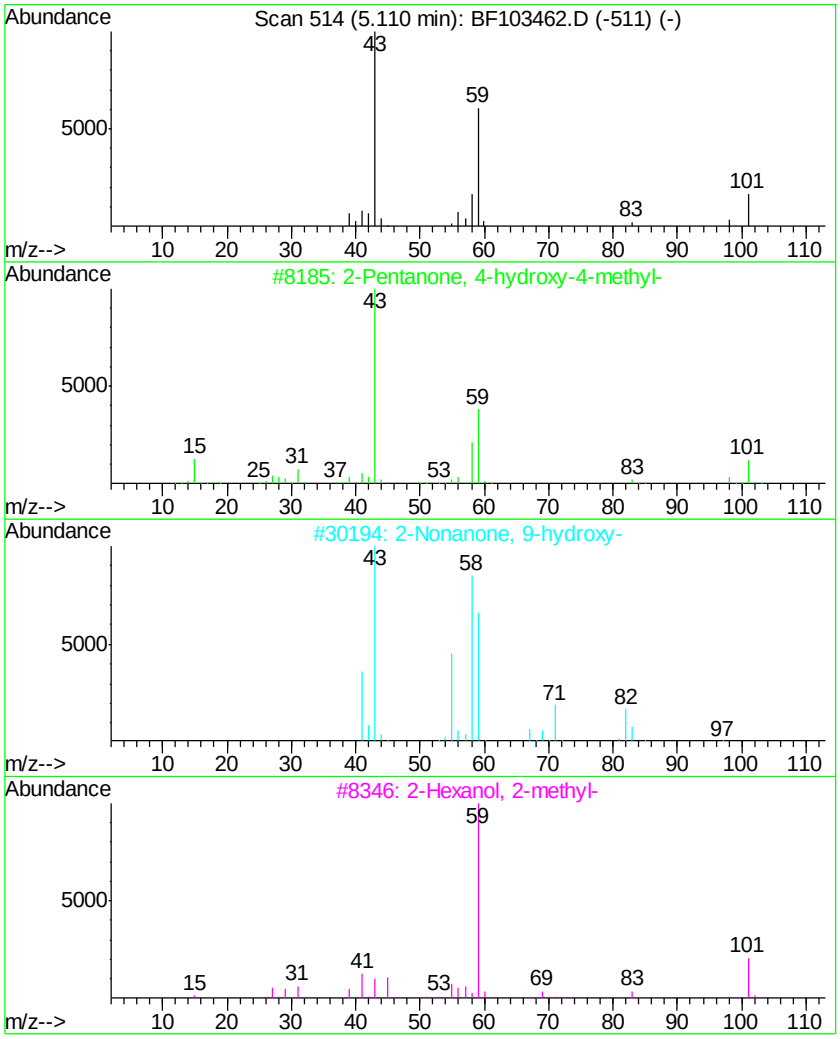
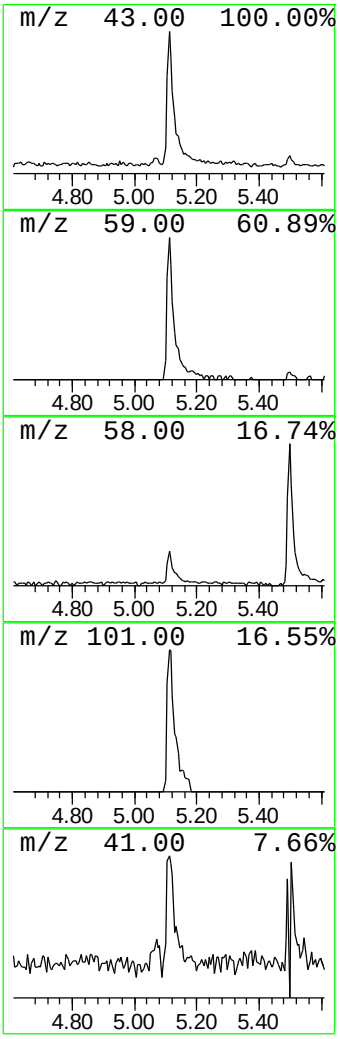
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	2.02 ng	98246	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	50
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103462.D
Acq On : 6 Mar 2018 18:23
Operator : SJ/JU
Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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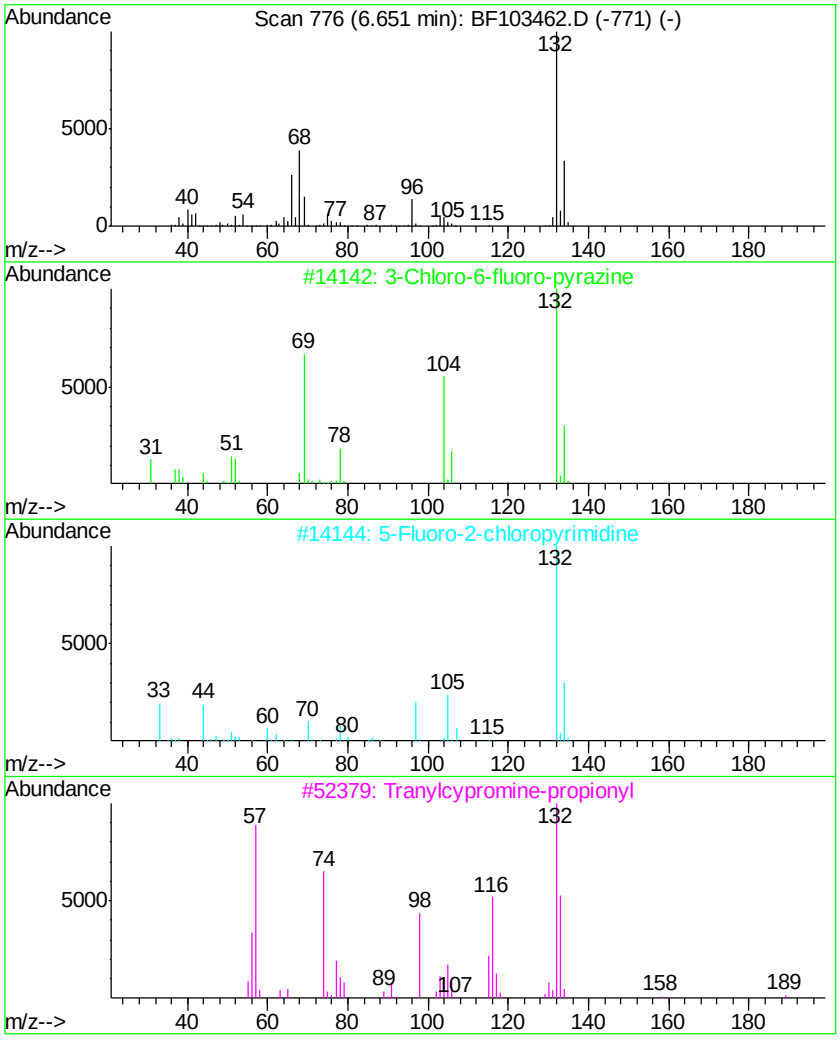
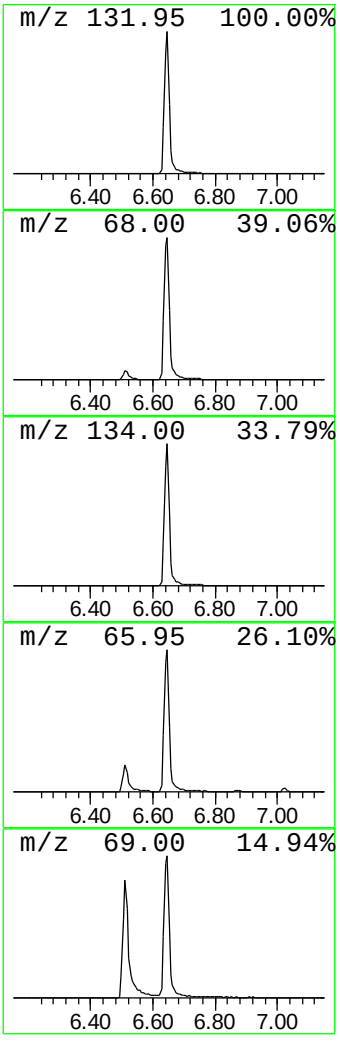
Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	66.73 ng	3245270	1,4-Dichlorobenzene-d4	6.87

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	Xenon	132	Xe	007440-63-3	9





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

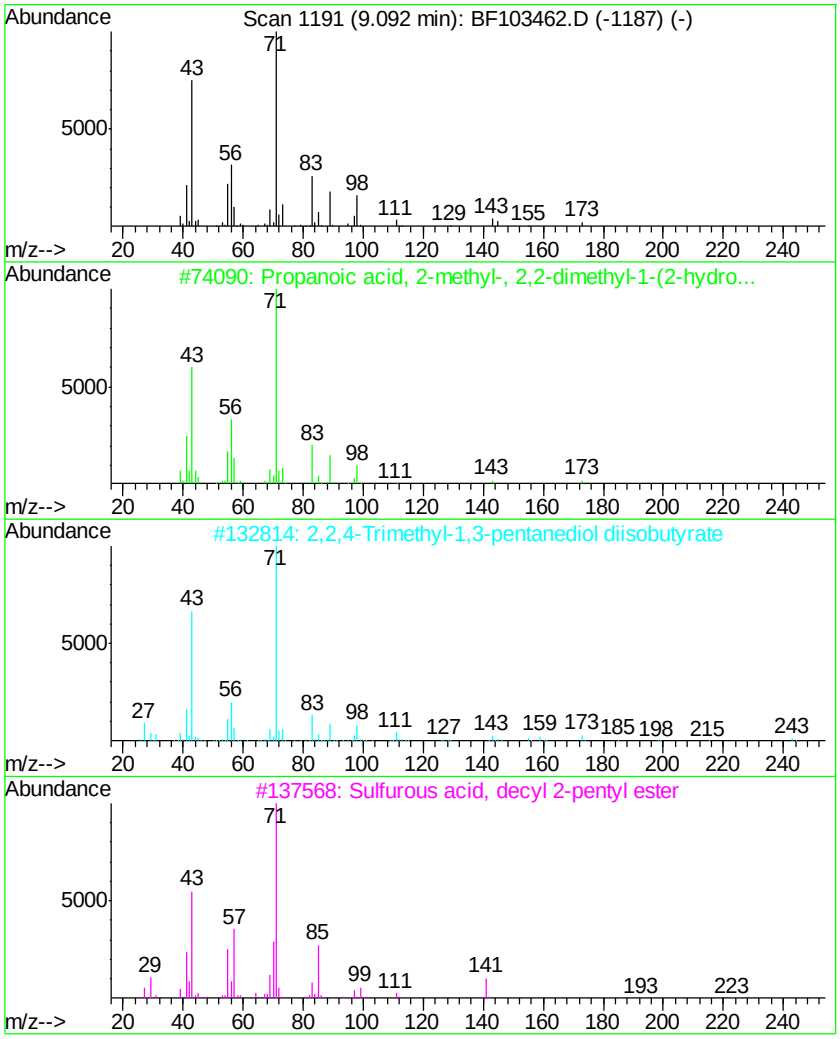
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

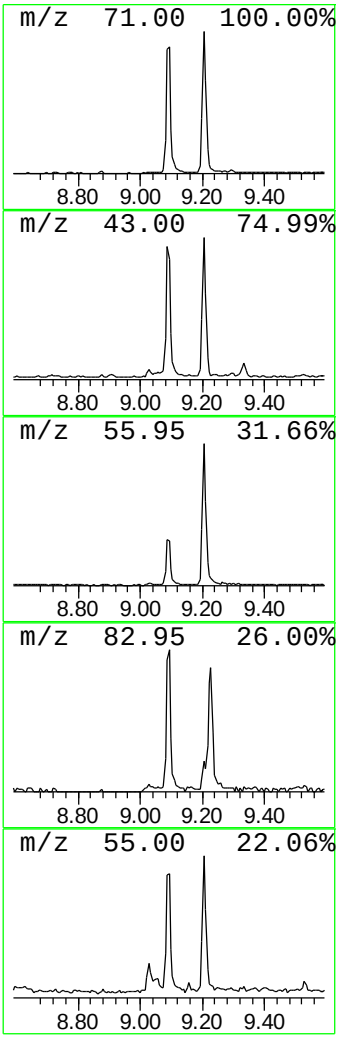
****

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	4.01 ng	258129	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	83
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	59
3	Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	43
4	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
5	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	40





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Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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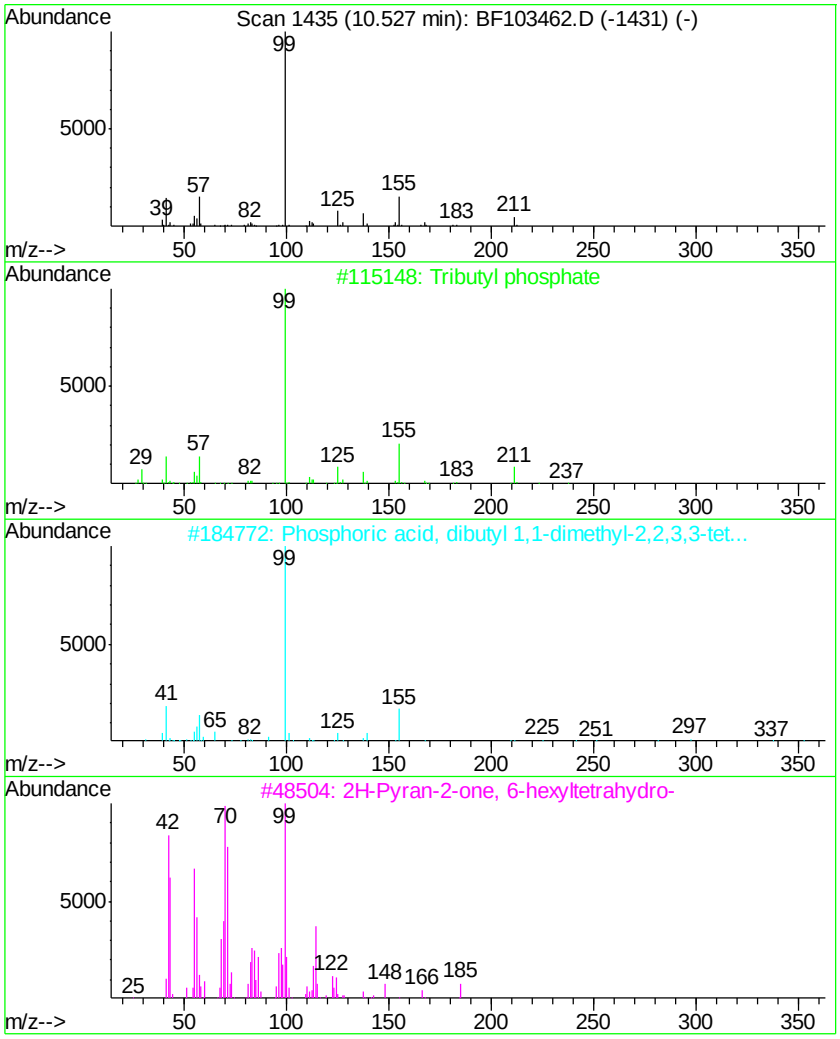
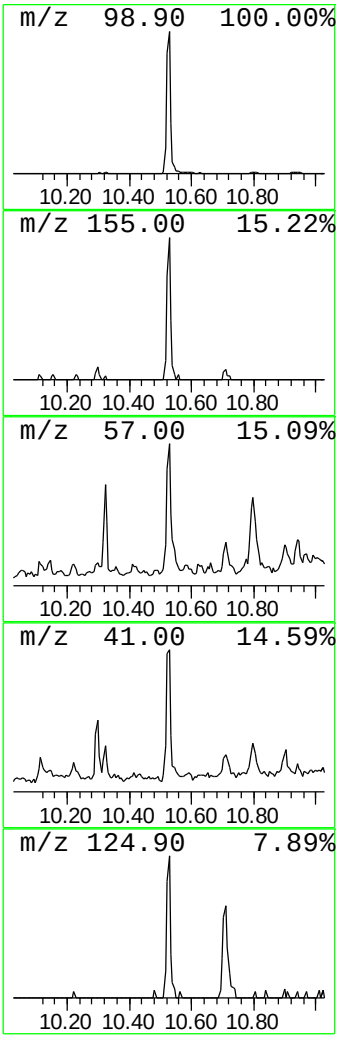
Peak Number 6 Tributyl phosphate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	2.55 ng	164434	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	91
2	Phosphoric acid, dibutyl 1,1-dim...	352	C13H25F4O4P	1000298-93-9	72
3	2H-Pyran-2-one, 6-hexyltetrahydro-	184	C11H20O2	000710-04-3	38
4	Bis(2-ethylhexyl)hydrogen phosphate	322	C16H35O4P	000298-07-7	36
5	(.+/-.)-Dethiobiotin	214	C10H18N2O3	000636-20-4	36





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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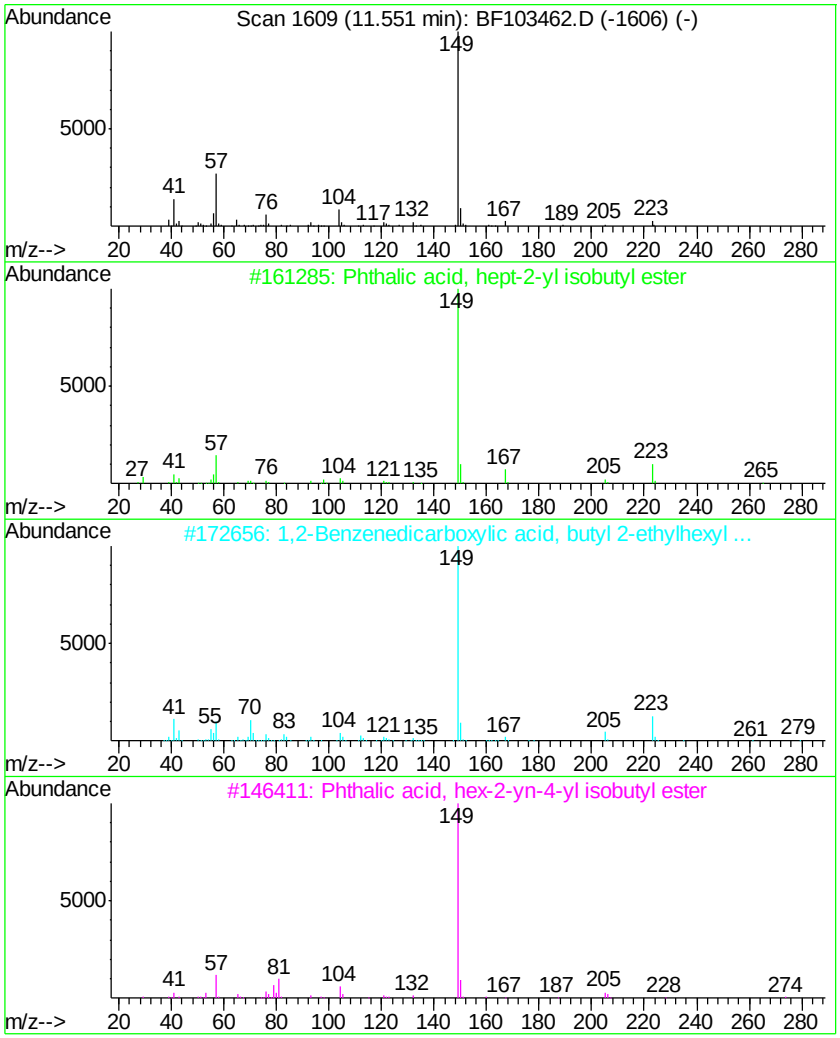
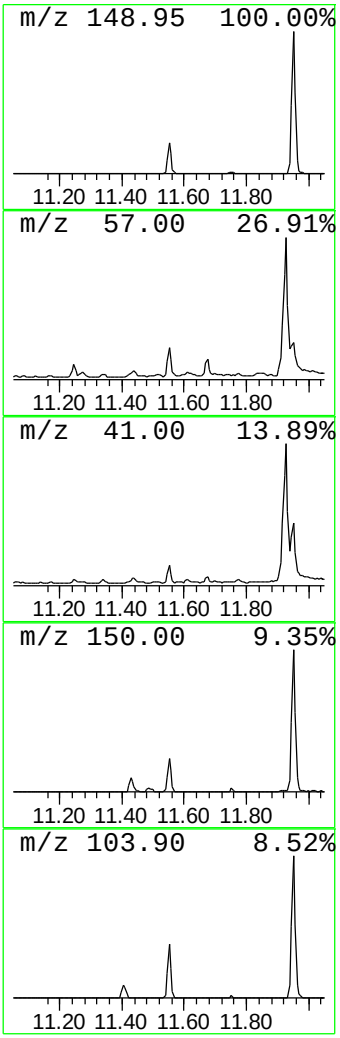
Peak Number 7 Phthalic acid, hept-2-yl is... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	2.84 ng	160653	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, hept-2-yl isobutyl...	320	C19H28O4	1000356-97-0	86
2	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	83
3	Phthalic acid, hex-2-yn-4-yl iso...	302	C18H22O4	1000315-19-9	78
4	Phthalic acid, cyclohexyl isohex...	304	C18H24O4	1000315-34-0	78
5	Phthalic acid, di(hept-3-yl) ester	362	C22H34O4	1000357-00-0	78





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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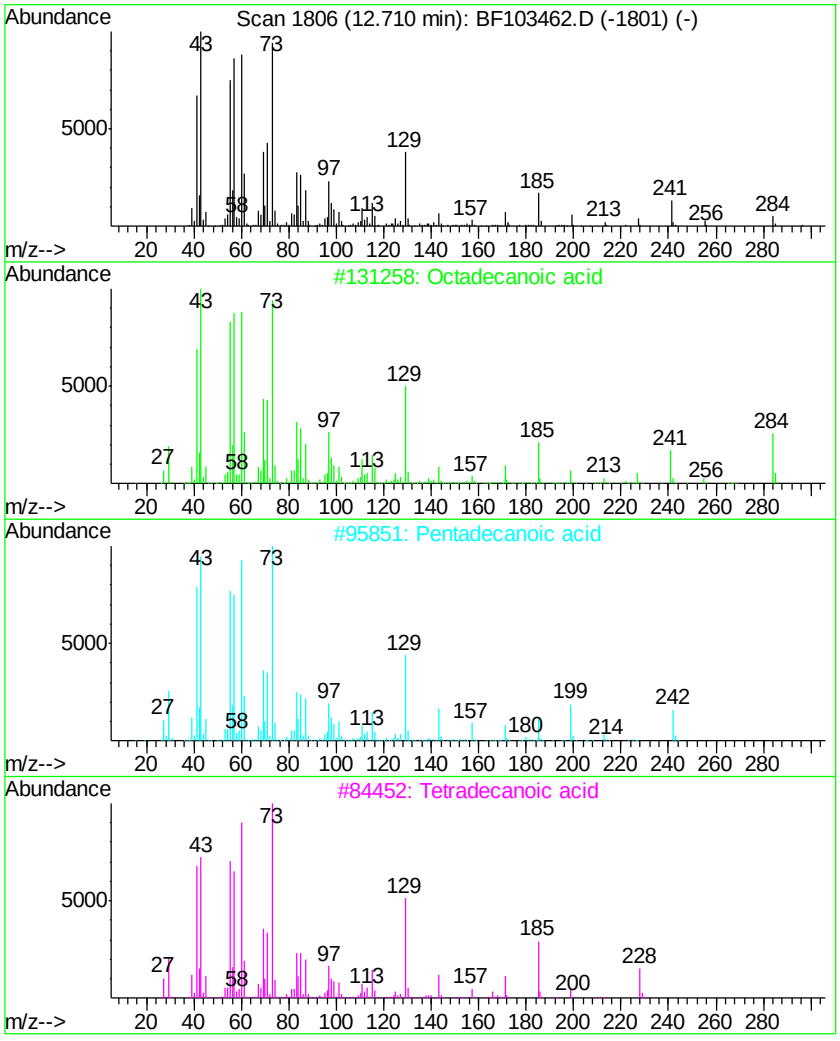
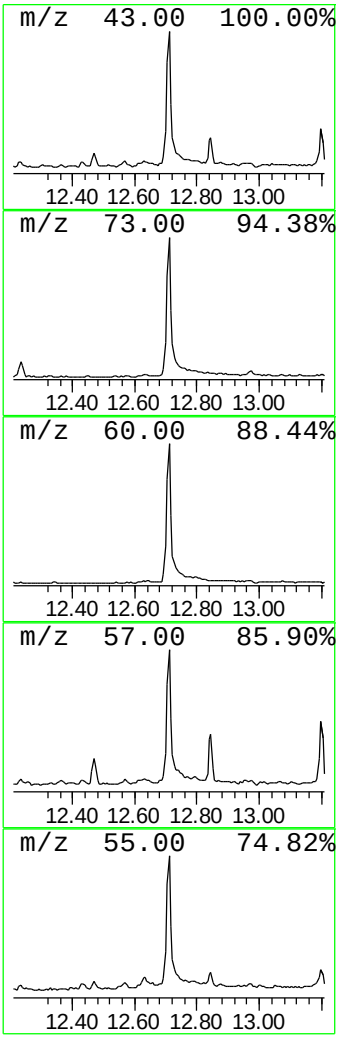
Peak Number 8 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	20.88 ng	1181950	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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Data File : BF103462.D
Acq On : 6 Mar 2018 18:23
Operator : SJ/JU
Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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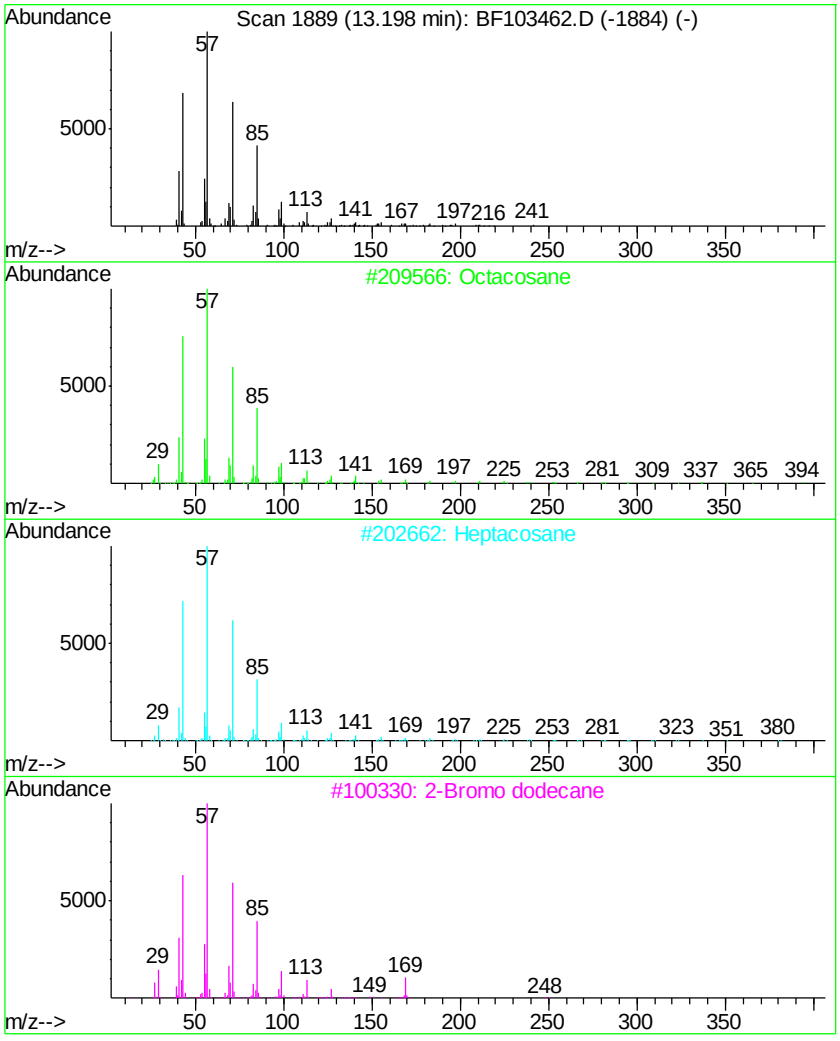
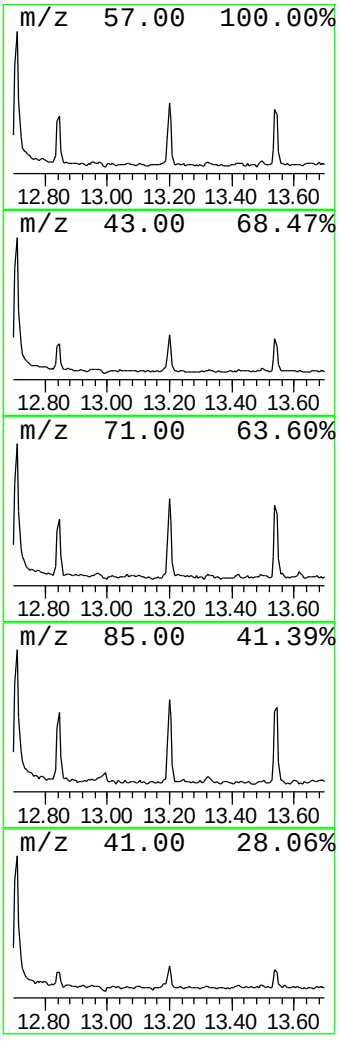
Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	4.71 ng	212144	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Pentadecane	212	C15H32	000629-62-9	87





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Data File : BF103462.D
Acq On : 6 Mar 2018 18:23
Operator : SJ/JU
Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

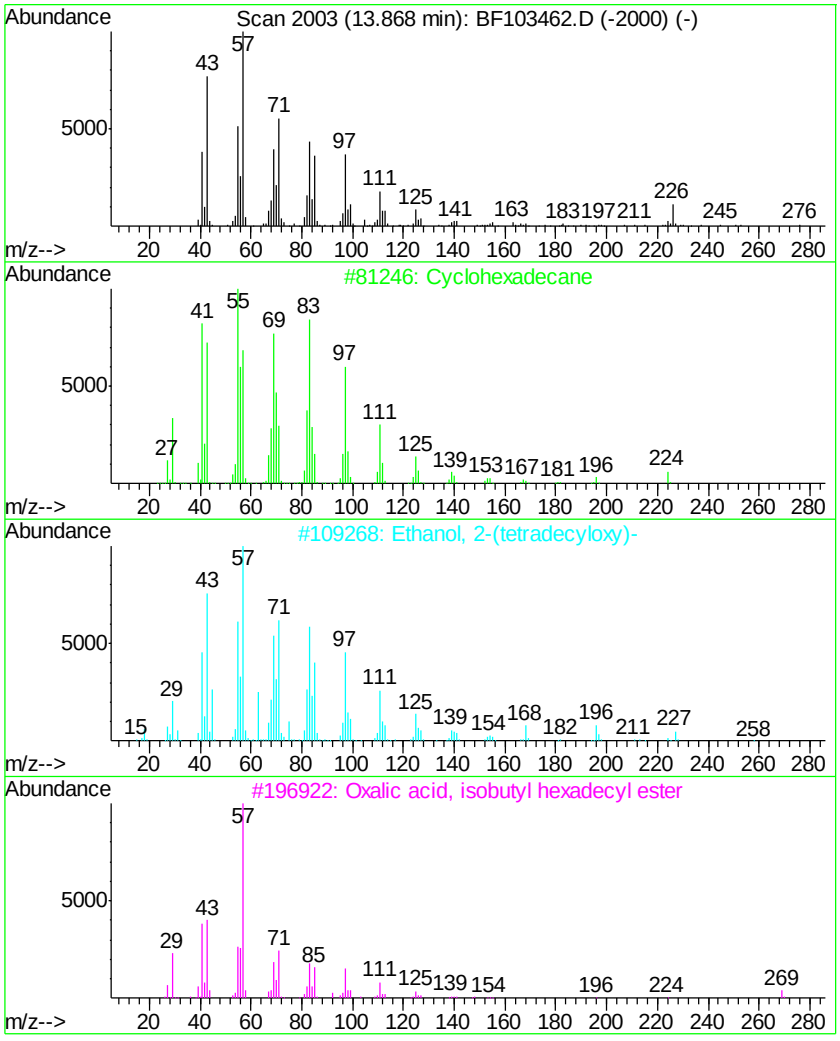
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

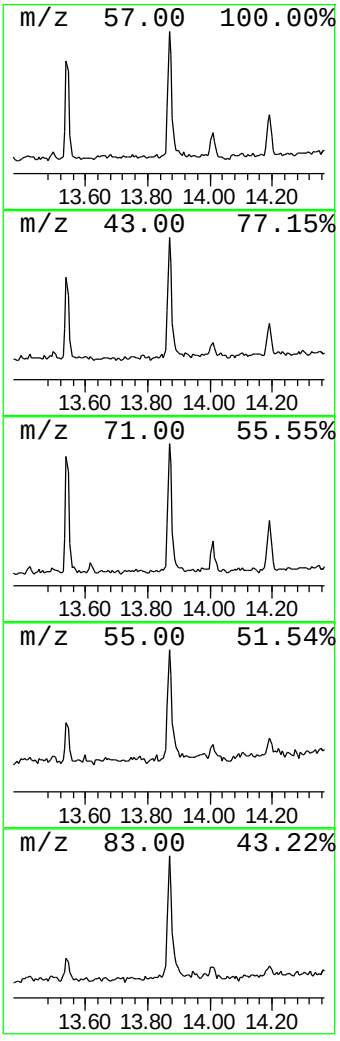
****

Peak Number 11 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	7.54 ng	339421	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	70
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	62





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF030618\
Data File : BF103462.D
Acq On : 6 Mar 2018 18:23
Operator : SJ/JU
Sample : J1792-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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	5.4	ng	263917	1	6.87	972649	20.0
2-Pentanone, 4-hy...	5.11	2.0	ng	98246	1	6.87	972649	20.0
unknown6.65	6.65	66.7	ng	3245270	1	6.87	972649	20.0
Propanoic acid, 2...	9.09	4.0	ng	258129	3	9.91	1287550	20.0
Tributyl phosphate	10.53	2.5	ng	164434	3	9.91	1287550	20.0
Phthalic acid, he...	11.55	2.8	ng	160653	4	11.40	1132210	20.0
Octadecanoic acid	12.71	20.9	ng	1181950	4	11.40	1132210	20.0
Octacosane	13.20	4.7	ng	212144	5	14.06	900230	20.0
Cyclohexadecane	13.87	7.5	ng	339421	5	14.06	900230	20.0