LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116751.D
Acq On : 1 Sep 2019 19:09
Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

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-BF083019.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	5.457	568	573	578	rBV	1247311	1205603	24.65%	4.077%
2	6.469	741	745	751	rBV	1494648	1412910	28.89%	4.778%
3	6.610	765	769	773	rBV	1527618	1357563	27.75%	4.591%
4	6.845	805	809	812	rBV	540854	437701	8.95%	1.480%
5	6.998	832	835	839	rBV	1133345	1035111	21.16%	3.501%
6	7.398	899	903	906	rBV	1019261	825312	16.87%	2.791%
7	8.128	1023	1027	1030	rBV	712585	590204	12.07%	1.996%
8	8.510	1088	1092	1098	rBV	64733	65903	1.35%	0.223%
9	8.733	1126	1130	1136	rBV	448857	393599	8.05%	1.331%
10	8.839	1144	1148	1151	rVB	78719	62666	1.28%	0.212%
11	8.881	1151	1155	1162	rBV	200279	229194	4.69%	0.775%
12	9.198	1206	1209	1212	rBV	2126158	1665895	34.06%	5.634%
13	9.586	1272	1275	1282	rVB	229733	202792	4.15%	0.686%
14	9.880	1321	1325	1328	rBV	879750	765397	15.65%	2.589%
15	10.233	1381	1385	1392	rBV	159598	172672	3.53%	0.584%
16	10.586	1442	1445	1448	rBV	329343	299414	6.12%	1.013%
17	10.663	1454	1458	1461	rBV	1285857	1117438	22.85%	3.779%
18	11.363	1573	1577	1579	rBV	875499	875555	17.90%	2.961%
19	11.380	1579	1580	1583	rVB	180092	132211	2.70%	0.447%
20	11.892	1664	1667	1669	rBV	701069	615211	12.58%	2.081%
21	11.922	1669	1672	1675	rVB	253235	242394	4.96%	0.820%
22	12.569	1779	1782	1785	rBV	545193	486440	9.94%	1.645%
23	12.674	1797	1800	1806	rBV	306166	337684	6.90%	1.142%
24	12.798	1819	1821	1824	rVB	470177	363520	7.43%	1.229%
25	12.945	1842	1846	1849	rBV	2059913	1829927	37.41%	6.189%
26	13.486	1934	1938	1941	rBV	1606389	1375656	28.12%	4.652%
27	13.839	1995	1998	2007	rVB3	333155	490090	10.02%	1.657%
28	13.980	2018	2022	2027	rBV2	4815198	4891345	100.00%	16.542%
29	14.380	2087	2090	2093	rVB	452456	385578	7.88%	1.304%
30	14.474	2102	2106	2109	rVV2	667314	635938	13.00%	2.151%
31	14.521	2109	2114	2118	rVV	2176697	2241094	45.82%	7.579%
32	14.574	2120	2123	2132	rVB2	409947	453542	9.27%	1.534%
33	14.674	2138	2140	2145	rBV5	92776	93760	1.92%	0.317%
34	15.021	2195	2199	2209	rBV	344670	624260	12.76%	2.111%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116751.D
Acq On : 1 Sep 2019 19:09
Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

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-BF083019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.104	2210	2213	2215	rBV	102737	106524	2.18%	0.360%
36	15.321	2247	2250	2255	rVB	208944	265087	5.42%	0.897%
37	15.380	2257	2260	2264	rVB	207257	224551	4.59%	0.759%
38	15.445	2267	2271	2274	rBV	513269	597525	12.22%	2.021%
39	15.910	2347	2350	2355	rVB3	63584	85631	1.75%	0.290%
40	16.880	2511	2515	2522	rVB2	110713	205949	4.21%	0.697%
41	17.315	2586	2589	2596	rVB2	99010	169760	3.47%	0.574%

Sum of corrected areas: 29568606

LSC Report - Integrated Chromatogram

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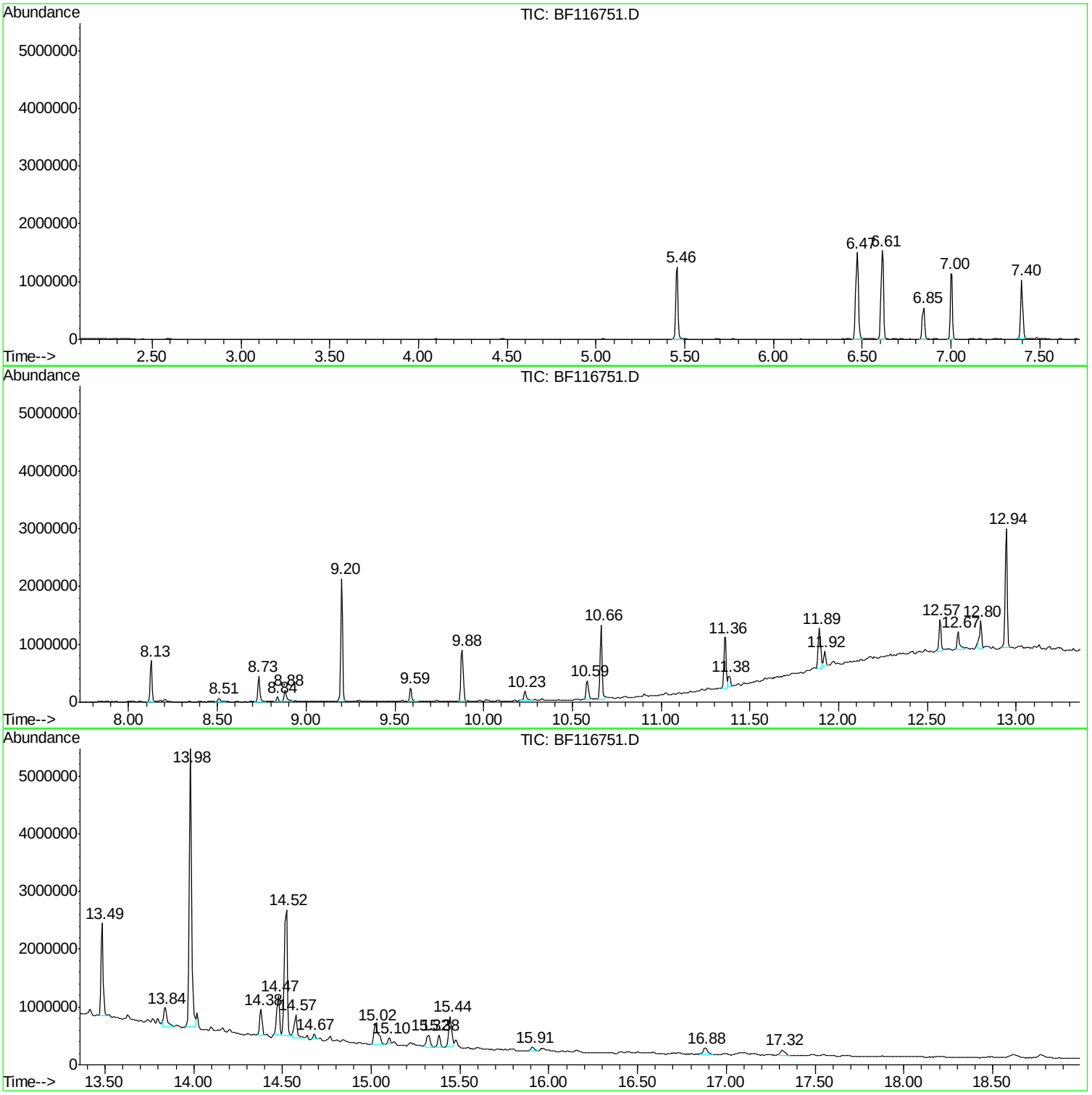
Data File : BF116751.D
Acq On : 1 Sep 2019 19:09
Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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\BF090119\
Data File : BF116751.D
Acq On : 1 Sep 2019 19:09
Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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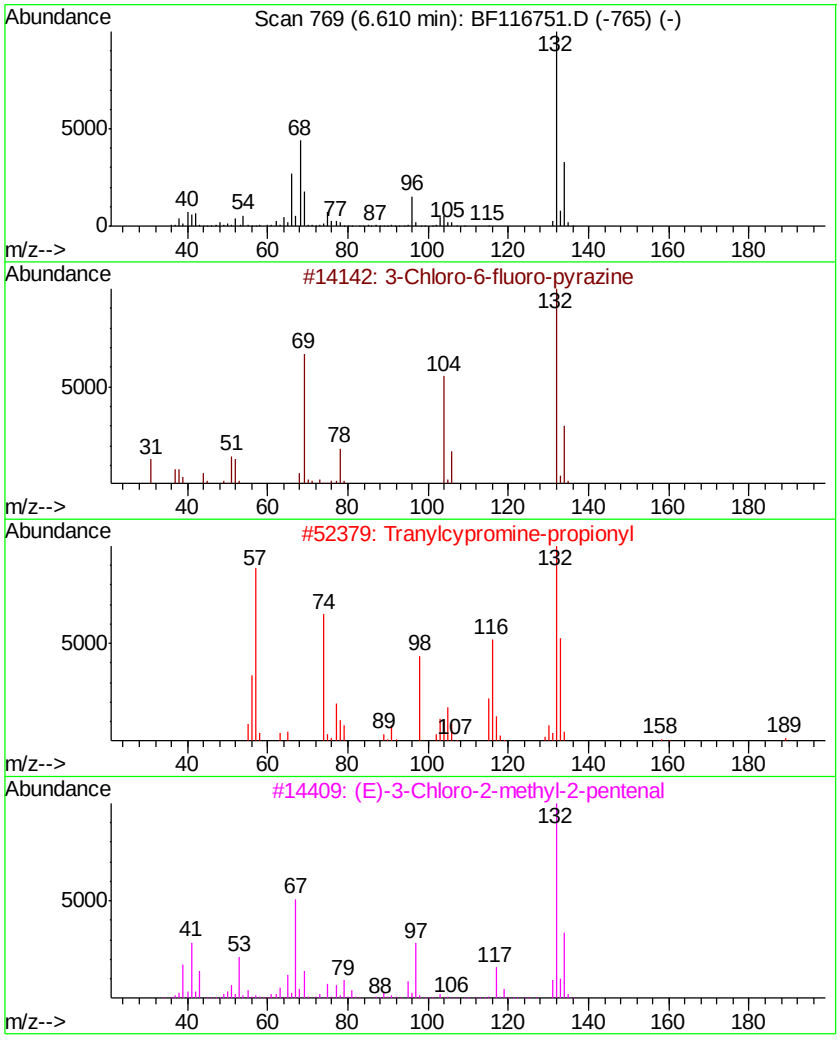
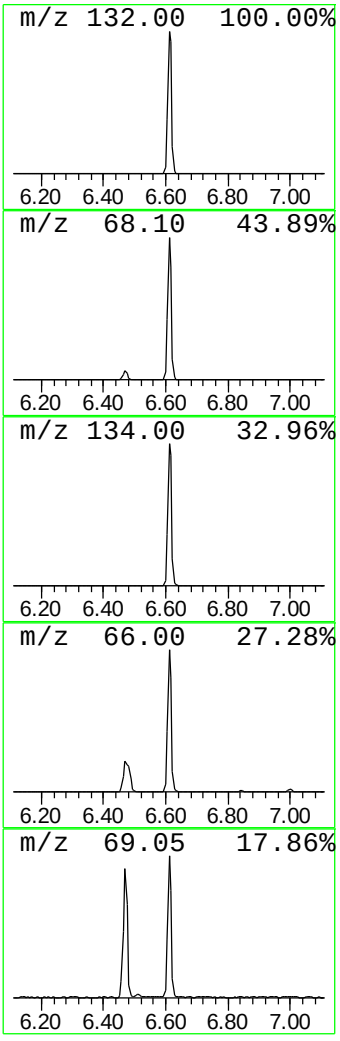
Peak Number 1 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	62.03 ng	1357560	1,4-Dichlorobenzene-d4	6.85

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	10
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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Data File : BF116751.D
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Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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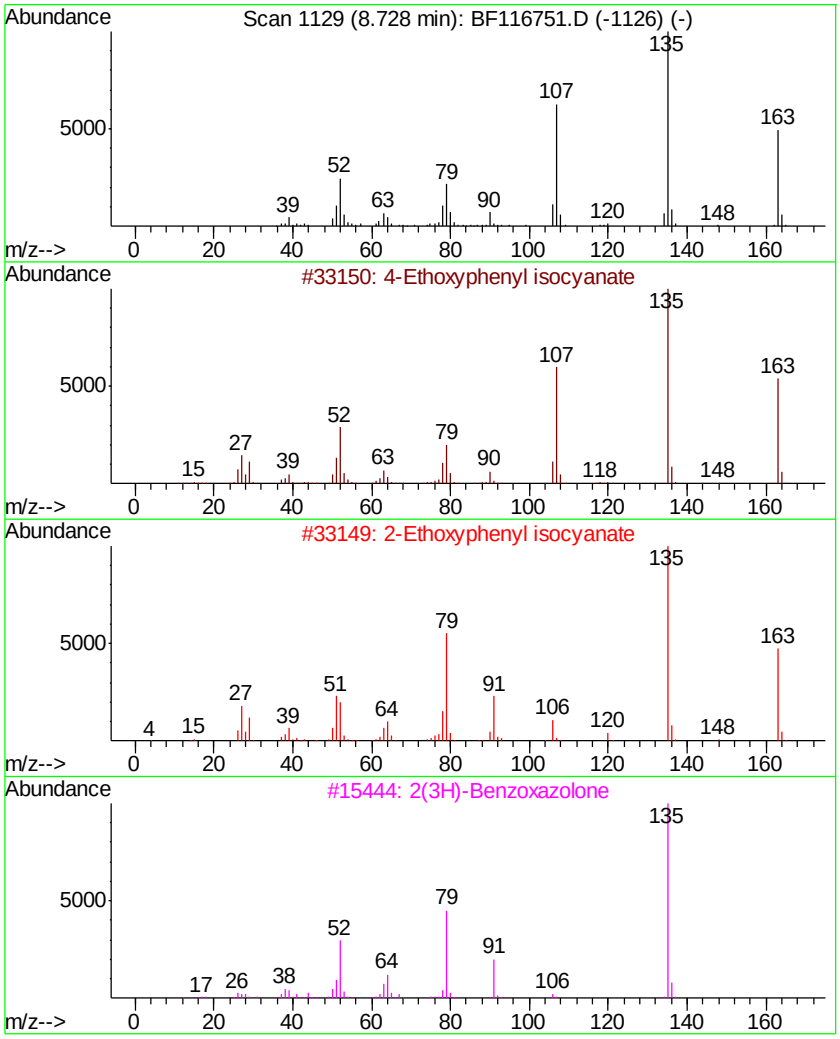
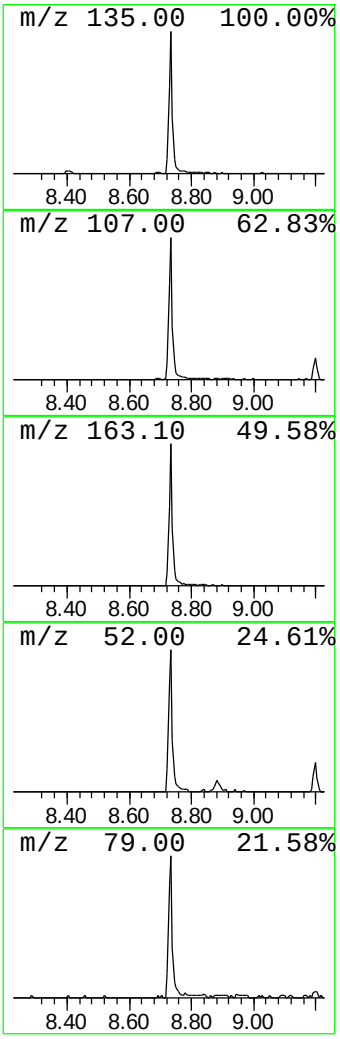
Peak Number 3 4-Ethoxyphenyl isocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	13.34 ng	393599	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Ethoxyphenyl isocyanate	163	C9H9NO2	032459-62-4	94
2	2-Ethoxyphenyl isocyanate	163	C9H9NO2	005395-71-1	72
3	2(3H)-Benzoxazolone	135	C7H5NO2	000059-49-4	47
4	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	47
5	2H-Imidazo[4,5-b]pyridin-2-one, ...	135	C6H5N3O	016328-62-4	42





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116751.D
Acq On : 1 Sep 2019 19:09
Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

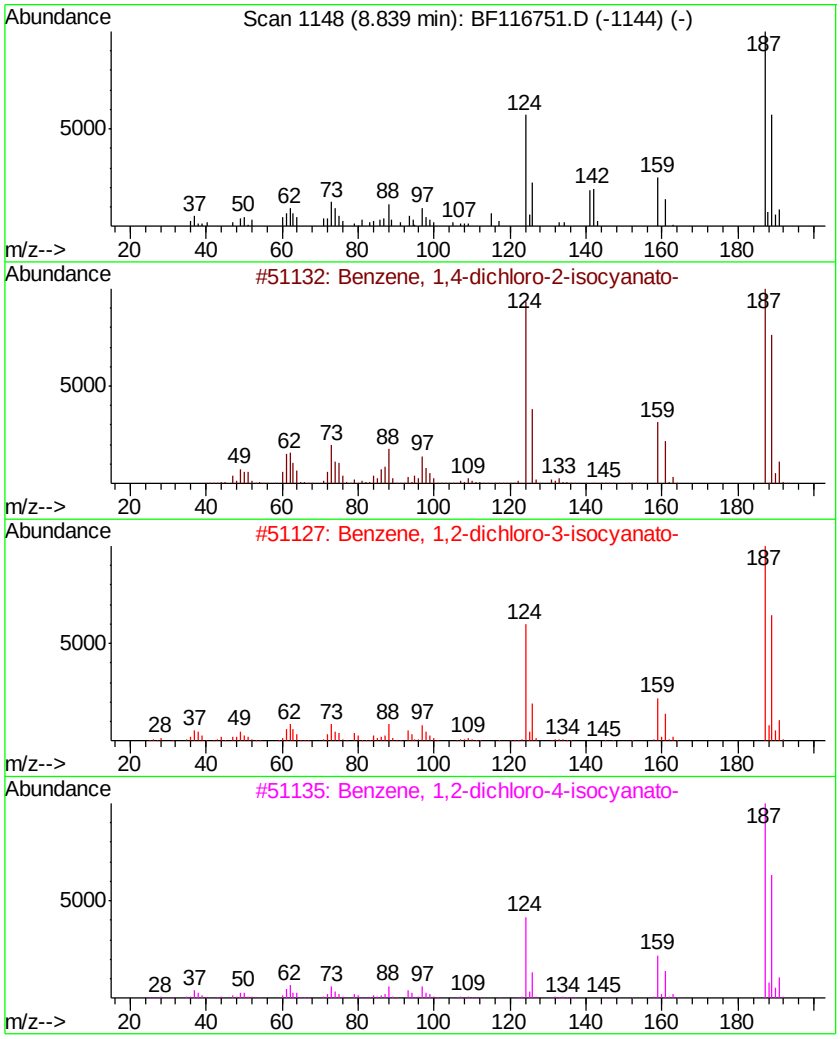
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

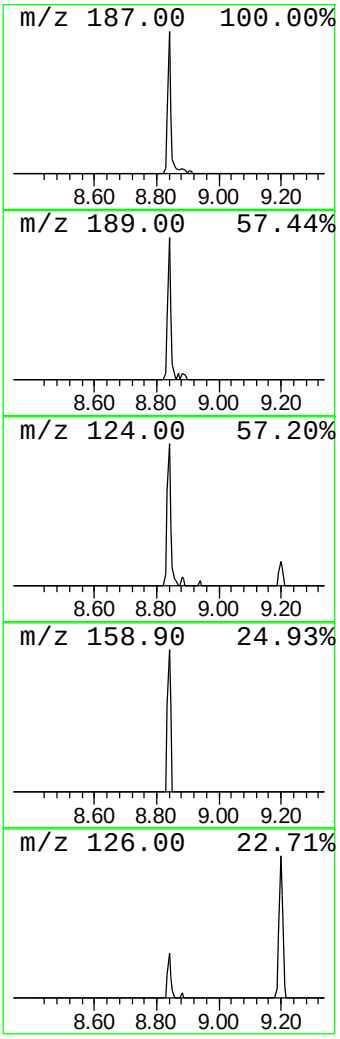
****

Peak Number 4 Benzene, 1,4-dichloro-2-iso... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.84	2.12 ng	62666	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-dichloro-2-isocyanato-	187	C7H3Cl2NO	005392-82-5	98
2	Benzene, 1,2-dichloro-3-isocyanato-	187	C7H3Cl2NO	041195-90-8	98
3	Benzene, 1,2-dichloro-4-isocyanato-	187	C7H3Cl2NO	000102-36-3	97
4	3,5-Dichlorophenyl isocyanate	187	C7H3Cl2NO	034893-92-0	96
5	Benzene, 1,3-dichloro-2-isocyanato-	187	C7H3Cl2NO	039920-37-1	96





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
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Acq On : 1 Sep 2019 19:09
Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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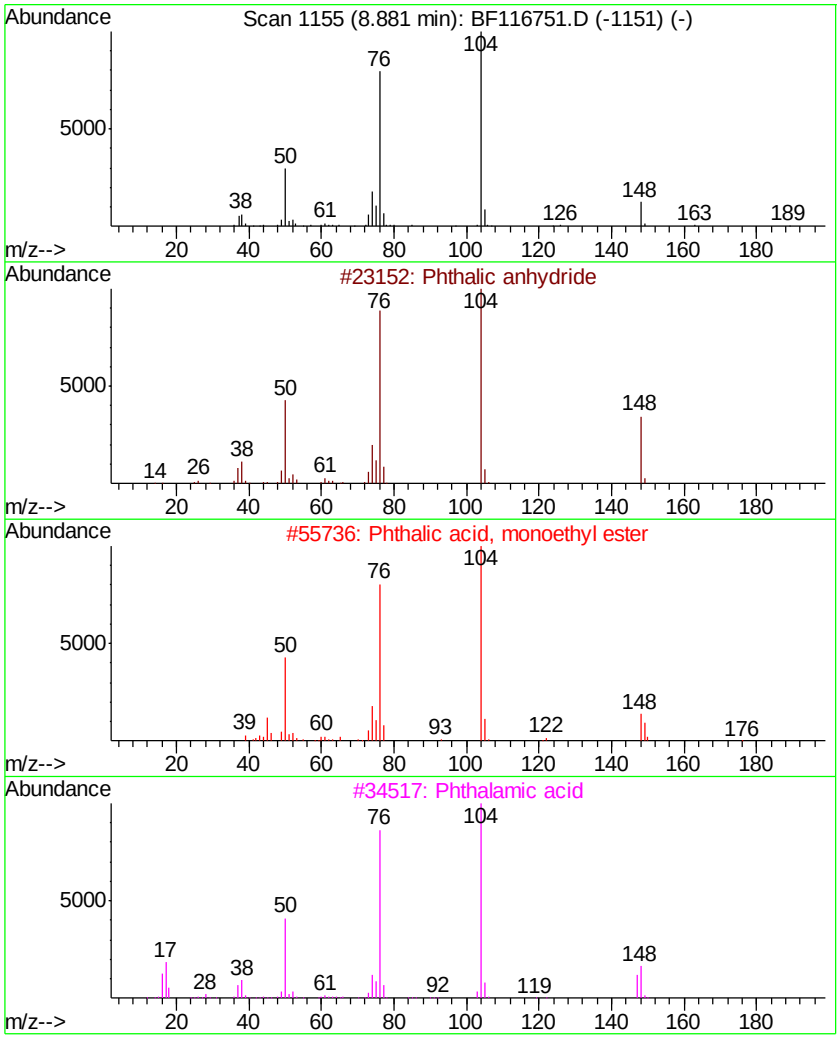
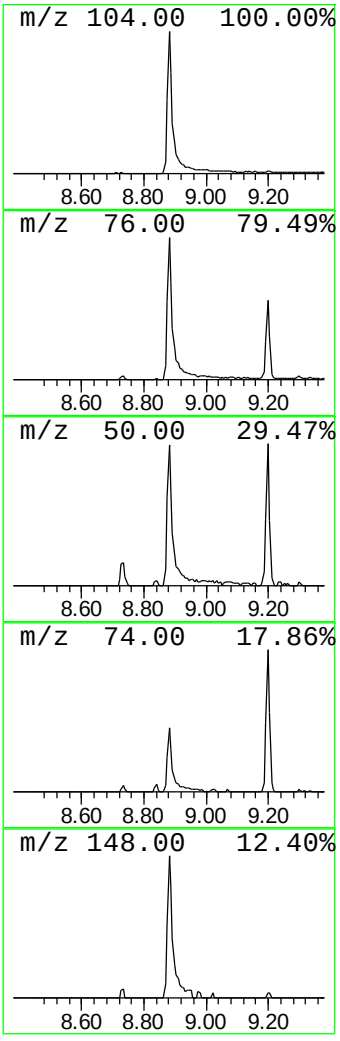
Peak Number 5 Phthalic anhydride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	7.77 ng	229194	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	95
2	Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	90
3	Phthalamic acid	165	C8H7NO3	000088-97-1	83
4	Ninhydrin	178	C9H6O4	000485-47-2	83
5	Indan-1,2,3-trione	160	C9H4O3	000938-24-9	83





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Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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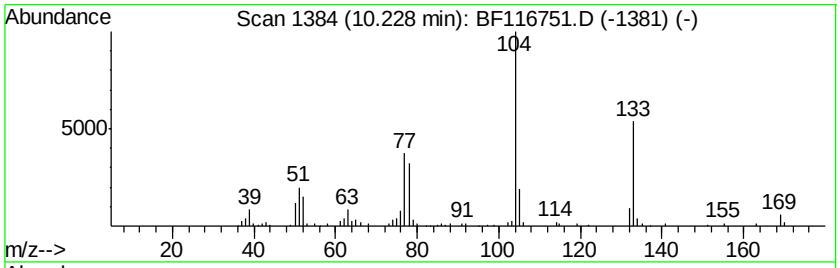
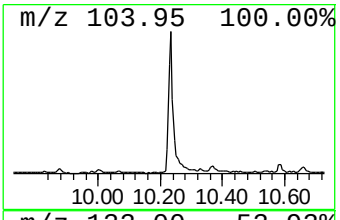
****

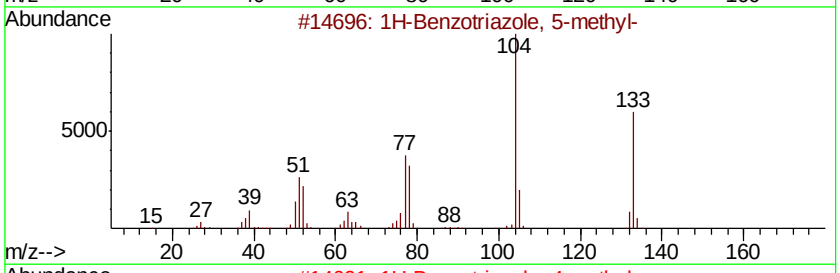
Peak Number 6 1H-Benzotriazole, 5-methyl- Concentration Rank 9

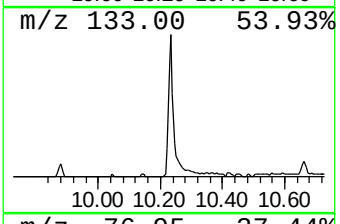
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.23	4.51 ng	172672	Acenaphthene-d10	9.88

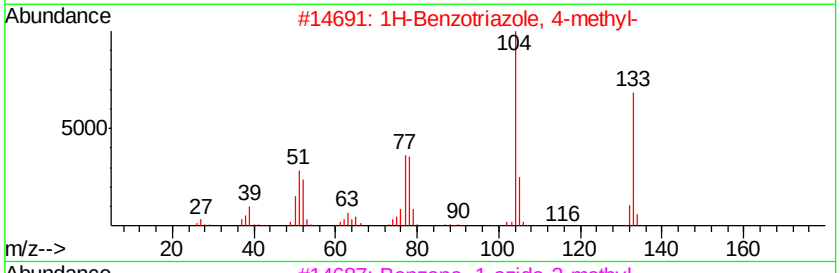
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	96
2	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	95
3	Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	64
4	Styrene	104	C8H8	000100-42-5	62
5	1H-Indol-5-ol	133	C8H7NO	001953-54-4	58

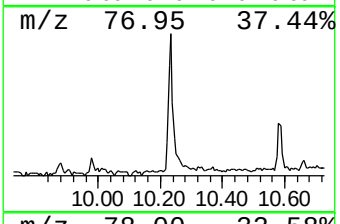


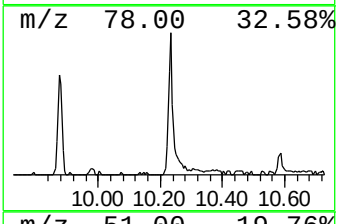


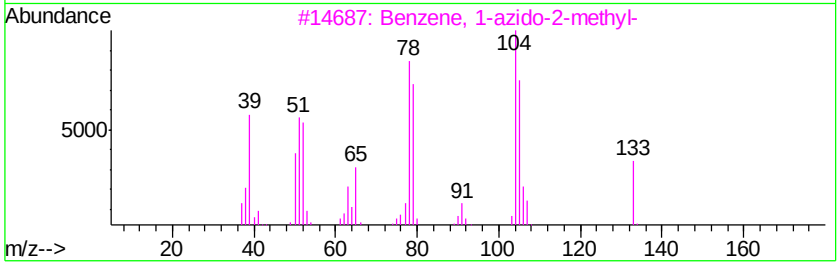


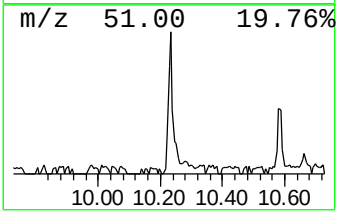












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

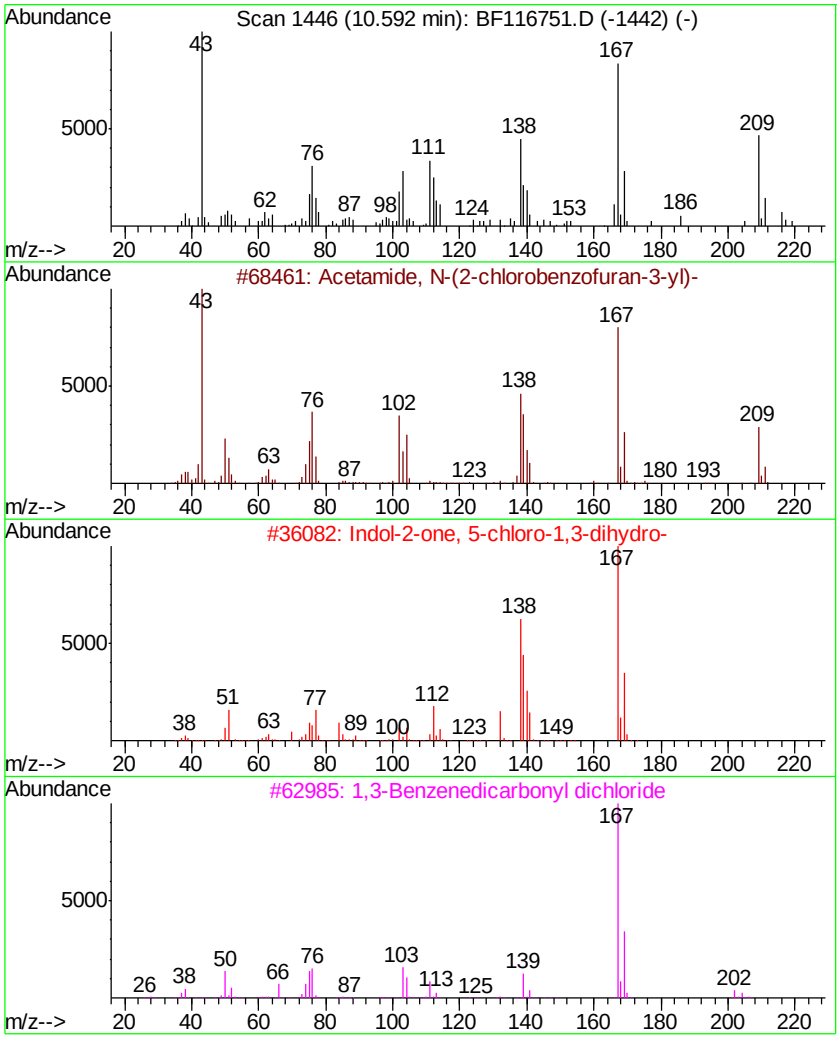
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

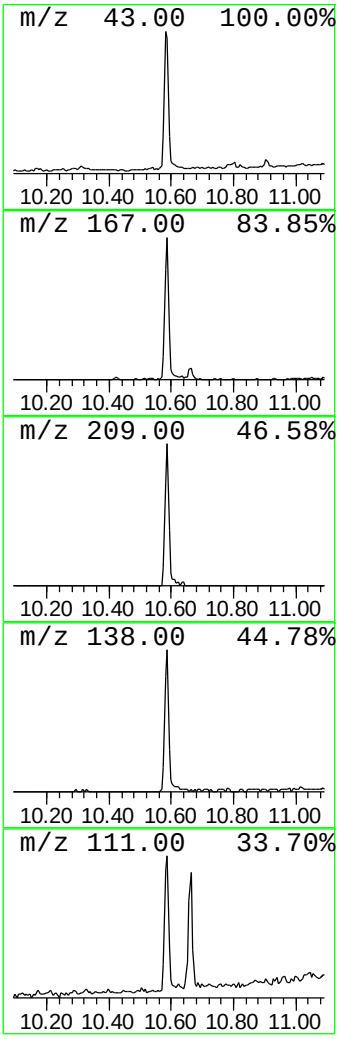
****

Peak Number 7 Acetamide, N-(2-chlorobenzo... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	7.82 ng	299414	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2-chlorobenzofuran...	209	C10H8ClNO2	067382-11-0	62
2	Indol-2-one, 5-chloro-1,3-dihydro-	167	C8H6ClNO	017630-75-0	45
3	1,3-Benzenedicarbonyl dichloride	202	C8H4Cl2O2	000099-63-8	32
4	Purin-6-amine, 8-(1-methylethylt...	209	C8H11N5S	330982-99-5	27
5	1,4-Benzenedicarbonyl dichloride	202	C8H4Cl2O2	000100-20-9	16





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Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

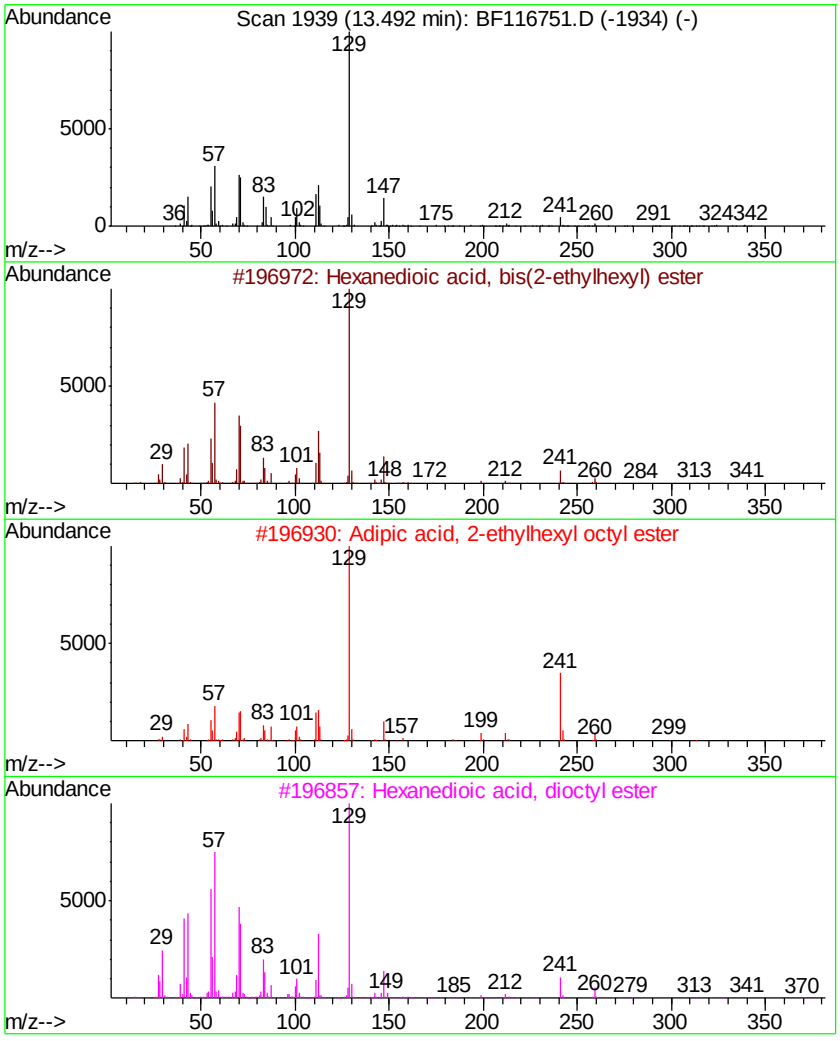
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

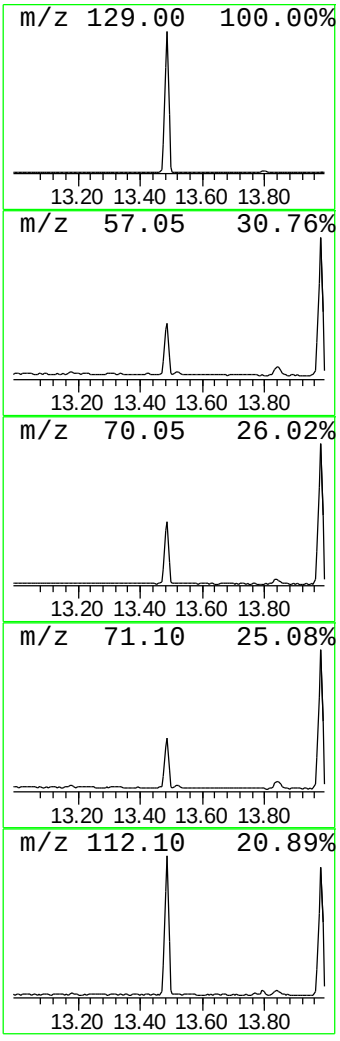
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexanedioic acid, bis(2-eth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	5.62 ng	1375660	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
3	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	86
4	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	53
5	Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116751.D
Acq On : 1 Sep 2019 19:09
Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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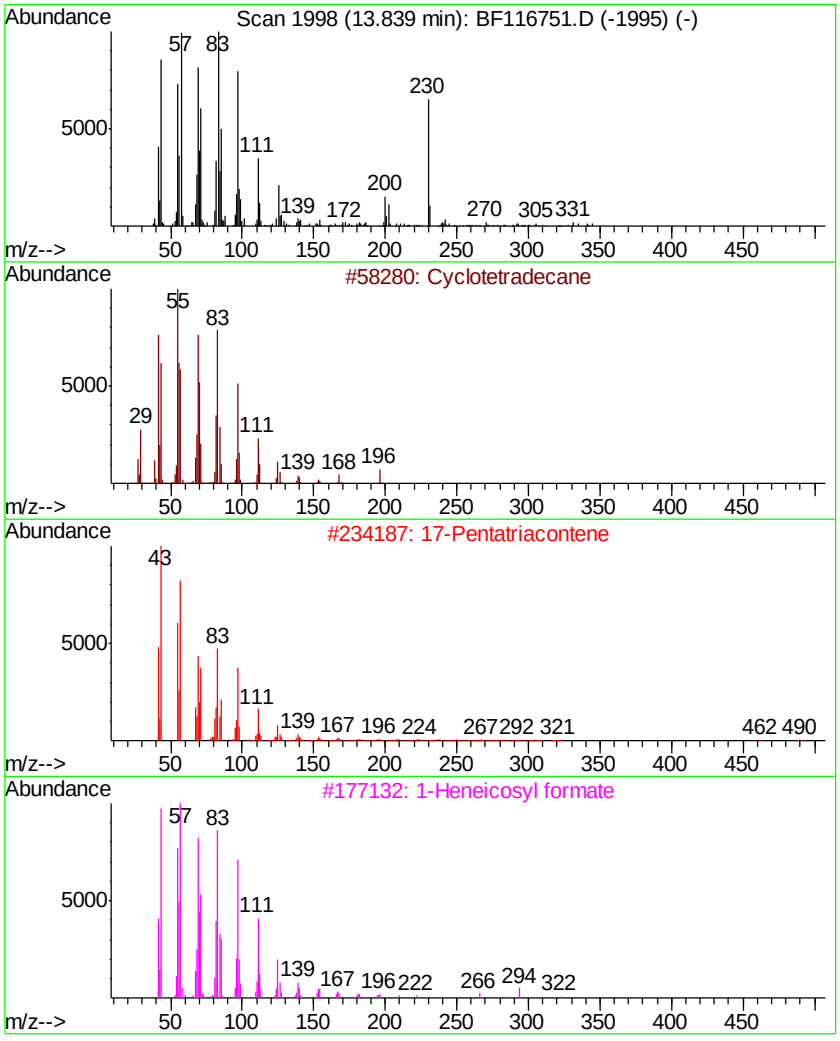
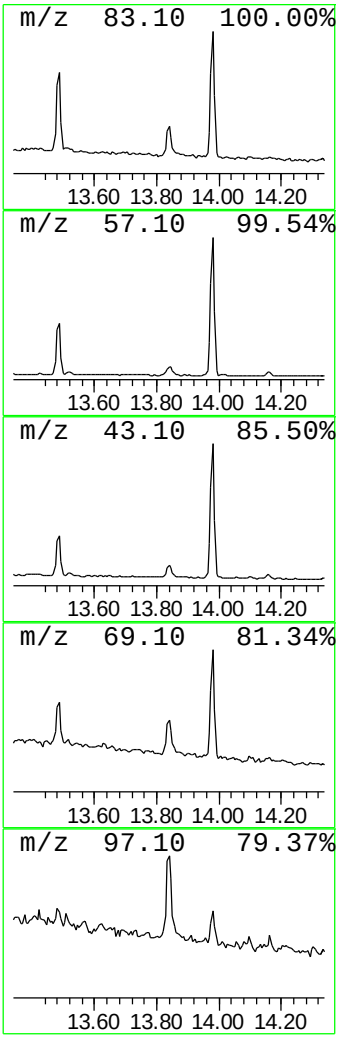
Peak Number 9 Cyclotetradecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	2.00 ng	490090	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	92
2	17-Pentatriacontene	491	C35H70	006971-40-0	90
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
5	Behenic alcohol	326	C22H46O	000661-19-8	81





Library Search Compound Report

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Operator : HP/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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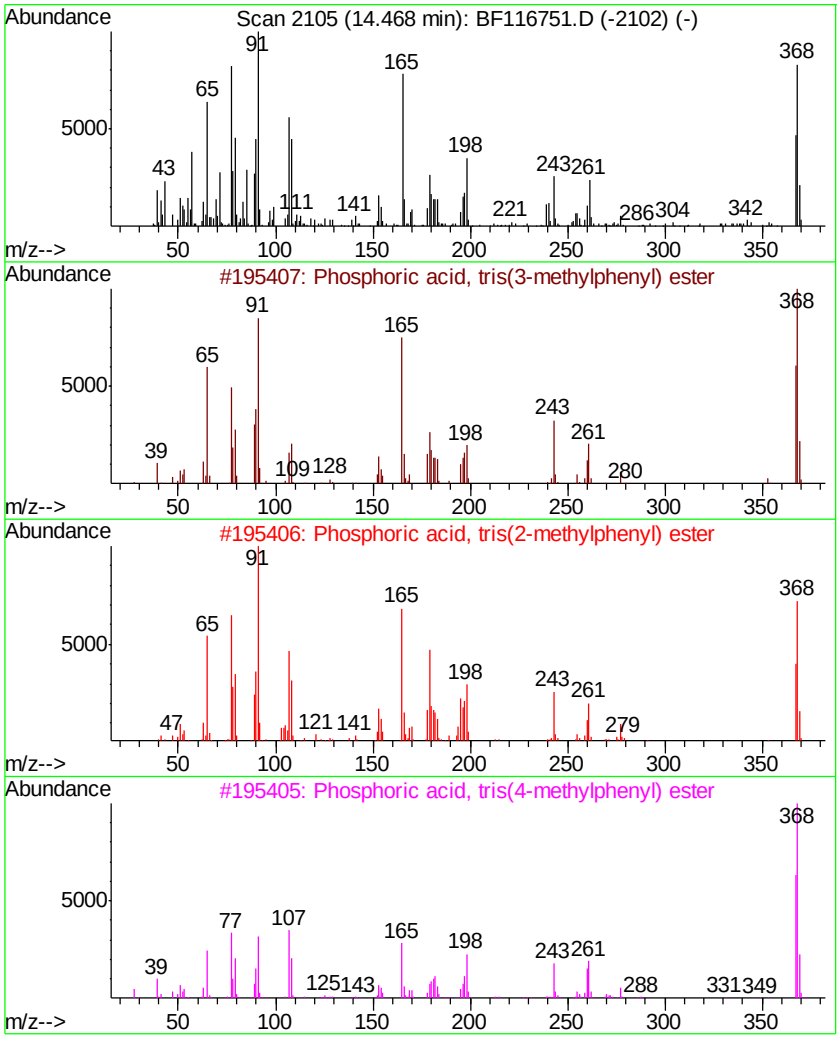
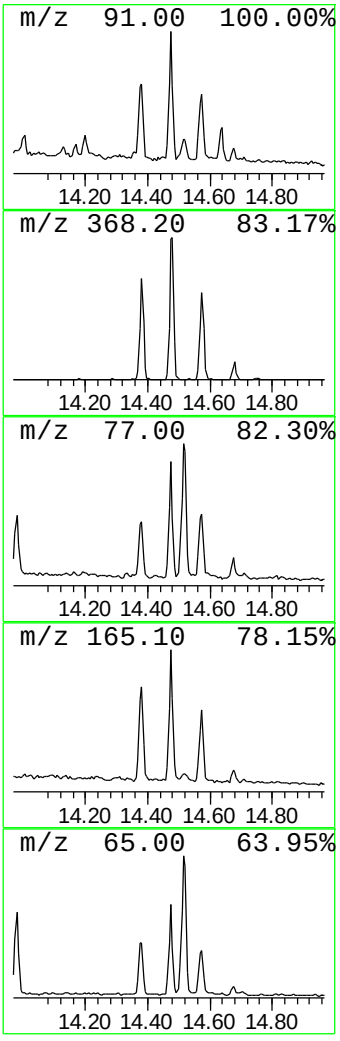
Peak Number 10 Phosphoric acid, tris(3-met... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.60 ng	635938	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphoric acid, tris(3-methylph...	368	C21H21O4P	000563-04-2	99
2	Phosphoric acid, tris(2-methylph...	368	C21H21O4P	000078-30-8	96
3	Phosphoric acid, tris(4-methylph...	368	C21H21O4P	000078-32-0	90
4	Carbamic acid, (2-methylphenyl)-...	165	C9H11NO2	014983-92-7	35
5	1,3-Dihydro-1-hydroxy-3,3-dimeth...	254	C17H18O2	007002-47-3	25





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Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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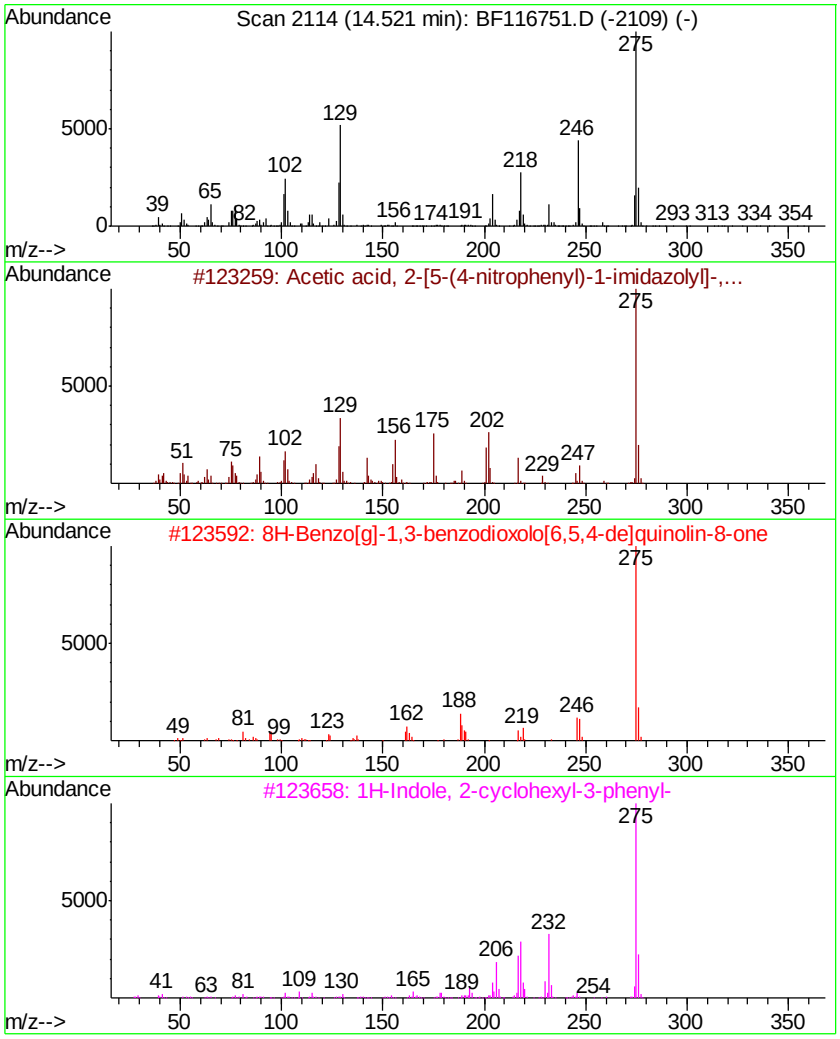
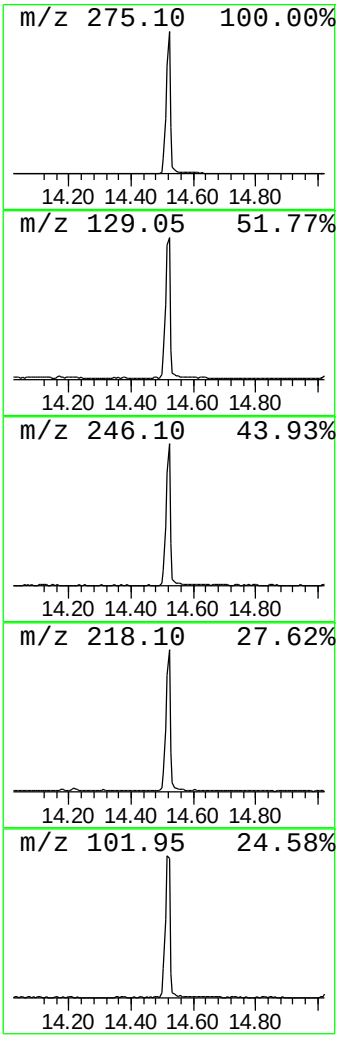
Peak Number 11 unknown14.52 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	9.16 ng	2241090	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-[5-(4-nitrophenyl...	275	C13H13N3O4	351064-45-4	49
2	8H-Benzo[g]-1,3-benzodioxolo[6,5...	275	C17H9NO3	000475-75-2	38
3	1H-Indole, 2-cyclohexyl-3-phenyl-	275	C20H21N	1000163-87-0	35
4	1-Methyl-5'-phenylspiro(indoline...	275	C17H13N3O	015970-21-5	32
5	1H-Pyrazolo[4',3':5,6]pyrido[2,3...	275	C12H13N5O3	349496-02-2	27





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Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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TIC Library : C:\DATABASE\NIST11.L
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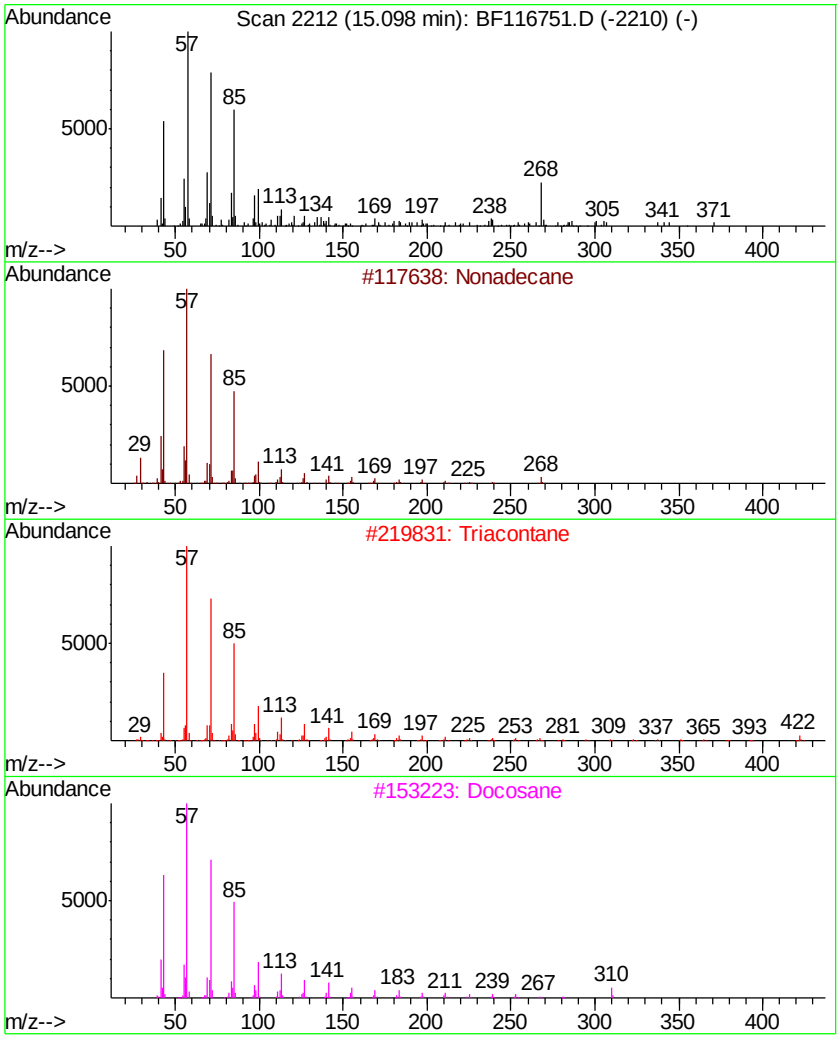
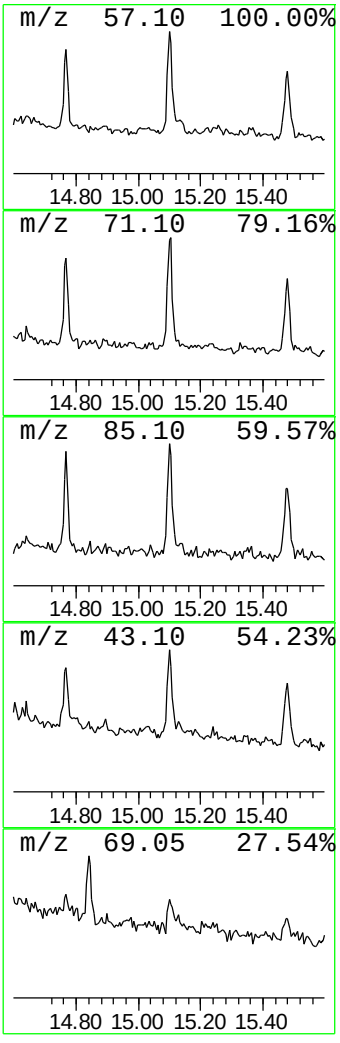
Peak Number 12 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	3.57 ng	106524	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	72
2	Triacontane	422	C30H62	000638-68-6	59
3	Docosane	310	C22H46	000629-97-0	59
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	58
5	Heneicosane	296	C21H44	000629-94-7	53





Library Search Compound Report

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Acq On : 1 Sep 2019 19:09
Operator : HP/JU
Sample : K4547-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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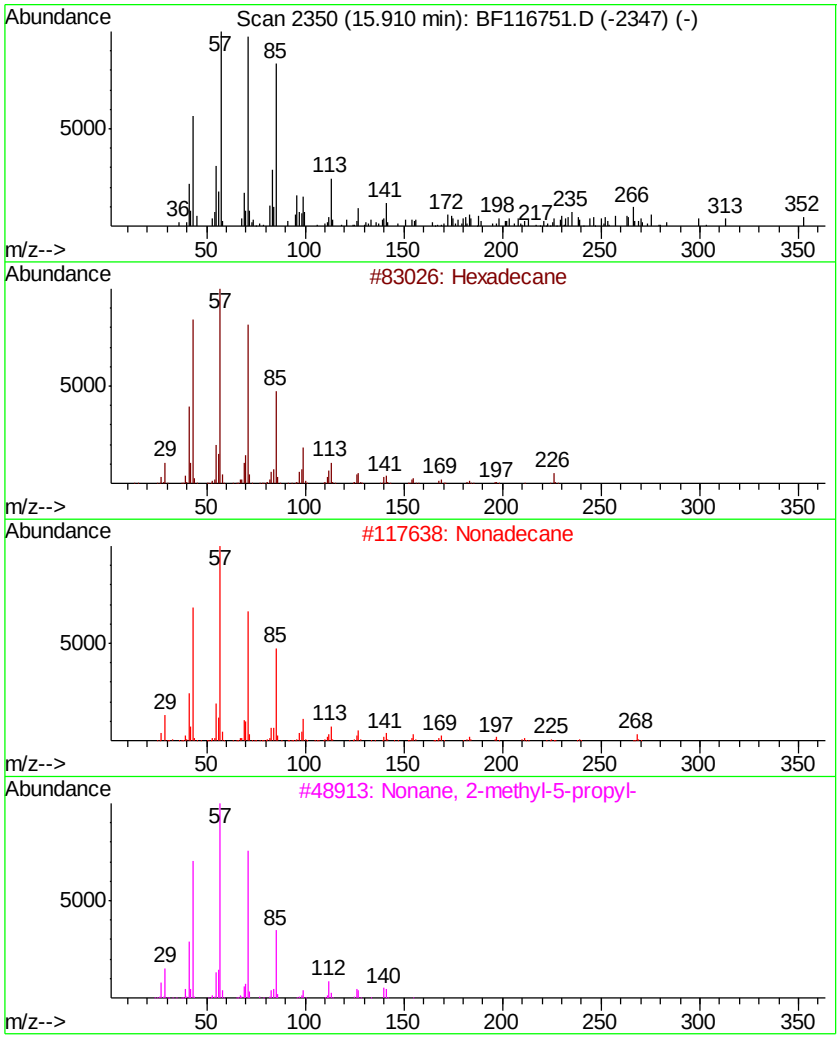
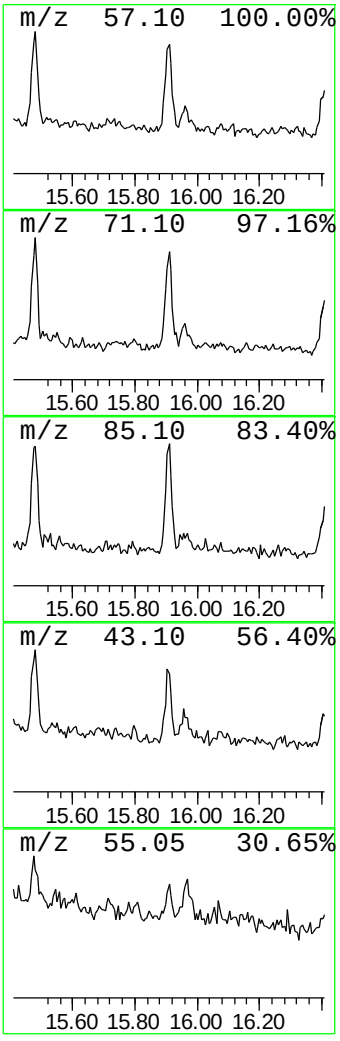
Peak Number 14 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.87 ng	85631	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	81
2	Nonadecane	268	C19H40	000629-92-5	64
3	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	59
4	Eicosane	282	C20H42	000112-95-8	59
5	Undecane, 3-methyl-	170	C12H26	001002-43-3	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090119\
Data File : BF116751.D
Acq On : 1 Sep 2019 19:09
Operator : HP/JU
Sample : K4547-04
Misc :
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Instrument : BNA_F
ClientSampleId : T3-S-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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
unknown6.61	6.61	62.0	ng	1357560	1	6.85	437701	20.0
4-Ethoxyphenyl is...	8.73	13.3	ng	393599	2	8.13	590204	20.0
Benzene, 1,4-dich...	8.84	2.1	ng	62666	2	8.13	590204	20.0
Phthalic anhydride	8.88	7.8	ng	229194	2	8.13	590204	20.0
1H-Benzotriazole,...	10.23	4.5	ng	172672	3	9.88	765397	20.0
Acetamide, N-(2-c...	10.59	7.8	ng	299414	3	9.88	765397	20.0
Hexanedioic acid,...	13.49	5.6	ng	1375660	5	13.99	4891350	20.0
Cyclotetradecane	13.84	2.0	ng	490090	5	13.99	4891350	20.0
Phosphoric acid, ...	14.47	2.6	ng	635938	5	13.99	4891350	20.0
unknown14.52	14.52	9.2	ng	2241090	5	13.99	4891350	20.0
Nonadecane	15.10	3.6	ng	106524	6	15.44	597525	20.0
Hexadecane	15.91	2.9	ng	85631	6	15.44	597525	20.0