LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
Data File : BF117597.D
Acq On : 29 Oct 2019 18:04
Operator : JU
Sample : K5541-13 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 15-70-(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-BF101819.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	4.910	477	480	497	rBV	34865	52532	13.95%	1.086%
2	5.357	553	556	570	rBV	174725	285874	75.93%	5.911%
3	5.557	586	590	595	rVB3	10093	11889	3.16%	0.246%
4	5.886	641	646	654	rVB2	3599	5332	1.42%	0.110%
5	6.328	717	721	728	rBB	4185	4745	1.26%	0.098%
6	6.404	731	734	749	rBV2	128102	336790	89.45%	6.964%
7	6.510	749	752	766	rVB	230106	376521	100.00%	7.786%
8	6.728	785	789	797	rBV	258040	235523	62.55%	4.870%
9	6.880	812	815	824	rBV	274277	270644	71.88%	5.596%
10	7.298	882	886	896	rBV	116096	173704	46.13%	3.592%
11	8.010	1004	1007	1020	rBV	234244	264301	70.20%	5.465%
12	8.851	1144	1150	1154	rBV2	3155	7309	1.94%	0.151%
13	9.080	1186	1189	1202	rBV	306839	299448	79.53%	6.192%
14	9.480	1254	1257	1265	rBV	38716	39362	10.45%	0.814%
15	9.757	1301	1304	1315	rBV	238166	245344	65.16%	5.073%
16	10.557	1437	1440	1450	rBV	119151	129723	34.45%	2.682%
17	10.627	1450	1452	1455	rVB	8818	7407	1.97%	0.153%
18	10.663	1455	1458	1459	rBV	5352	6152	1.63%	0.127%
19	10.686	1459	1462	1465	rVB	6947	7510	1.99%	0.155%
20	10.733	1468	1470	1473	rBV	17241	16929	4.50%	0.350%
21	10.763	1473	1475	1479	rVV2	15515	19986	5.31%	0.413%
22	10.798	1479	1481	1484	rVV2	14434	15723	4.18%	0.325%
23	10.821	1484	1485	1489	rVB	8396	6823	1.81%	0.141%
24	10.874	1489	1494	1498	rBV3	5427	10950	2.91%	0.226%
25	10.916	1498	1501	1504	rVB2	11354	13994	3.72%	0.289%
26	10.951	1504	1507	1510	rBV	15675	17752	4.71%	0.367%
27	10.986	1510	1513	1516	rVB3	10369	11037	2.93%	0.228%
28	11.110	1531	1534	1537	rVB	10107	9209	2.45%	0.190%
29	11.204	1546	1550	1554	rVB3	5233	6600	1.75%	0.136%
30	11.245	1554	1557	1561	rBV	220394	233725	62.07%	4.833%
31	11.333	1569	1572	1574	rBV2	4580	4187	1.11%	0.087%
32	11.774	1644	1647	1655	rBV4	53008	63447	16.85%	1.312%
33	11.857	1658	1661	1668	rVV2	29251	31066	8.25%	0.642%
34	11.915	1668	1671	1672	rVV	19538	17613	4.68%	0.364%

LSC Area Percent Report

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Operator : JU
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 15-70-(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-BF101819.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.939	1672	1675	1681	rVB	35447	46170	12.26%	0.955%
36	12.045	1688	1693	1699	rBV7	8499	18962	5.04%	0.392%
37	12.098	1699	1702	1705	rVB4	7778	9761	2.59%	0.202%
38	12.180	1714	1716	1720	rVB4	8649	5458	1.45%	0.113%
39	12.227	1720	1724	1728	rBV7	4562	6077	1.61%	0.126%
40	12.274	1728	1732	1734	rVB	12238	12619	3.35%	0.261%
41	12.304	1734	1737	1740	rBV4	9043	14777	3.92%	0.306%
42	12.362	1744	1747	1750	rVV2	20983	17913	4.76%	0.370%
43	12.462	1761	1764	1772	rBV	69518	74213	19.71%	1.535%
44	12.557	1777	1780	1785	rBV5	27205	34897	9.27%	0.722%
45	12.621	1788	1791	1793	rVB3	9265	9425	2.50%	0.195%
46	12.692	1798	1803	1805	rBV	71908	75262	19.99%	1.556%
47	12.721	1805	1808	1819	rVB	128703	189227	50.26%	3.913%
48	12.827	1822	1826	1831	rVB	341207	295792	78.56%	6.116%
49	12.968	1847	1850	1851	rBV3	10226	10364	2.75%	0.214%
50	13.015	1855	1858	1864	rVV4	15456	32338	8.59%	0.669%
51	13.104	1871	1873	1880	rBV7	11130	18128	4.81%	0.375%
52	13.298	1903	1906	1910	rBV2	88013	79572	21.13%	1.645%
53	13.857	1998	2001	2004	rBV	63226	67134	17.83%	1.388%
54	13.892	2004	2007	2011	rBV	252736	279550	74.25%	5.780%
55	15.333	2249	2252	2264	rVB	140797	233192	61.93%	4.822%
56	15.715	2314	2317	2323	rVB2	44543	66167	17.57%	1.368%

Sum of corrected areas: 4836149

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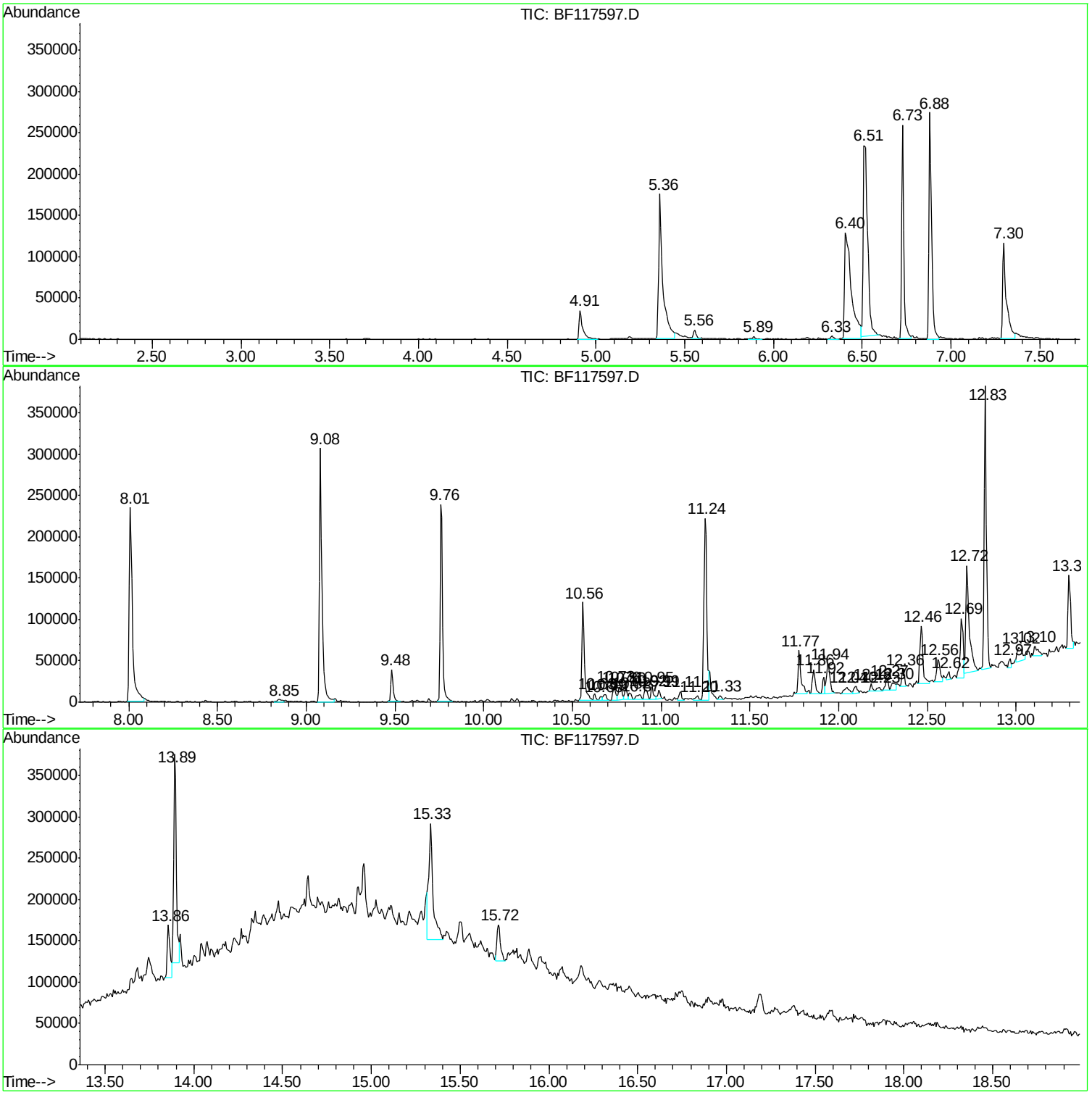
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
15-70-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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\BF102919\
Data File : BF117597.D
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

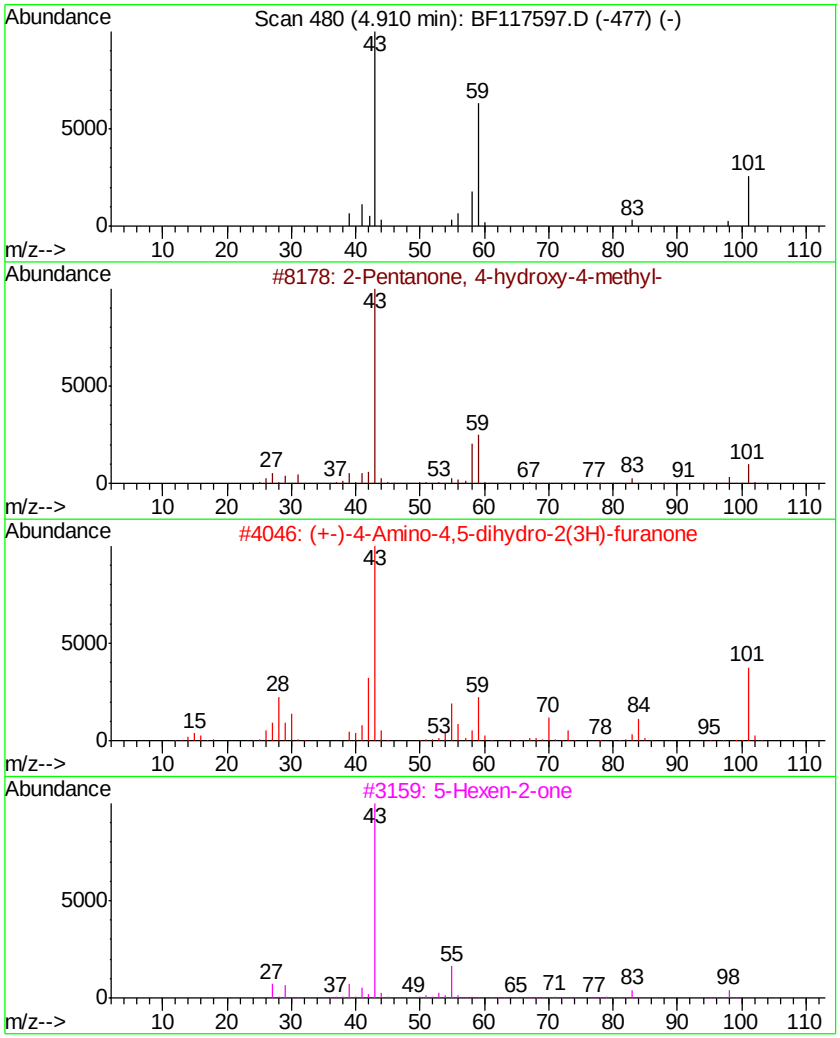
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

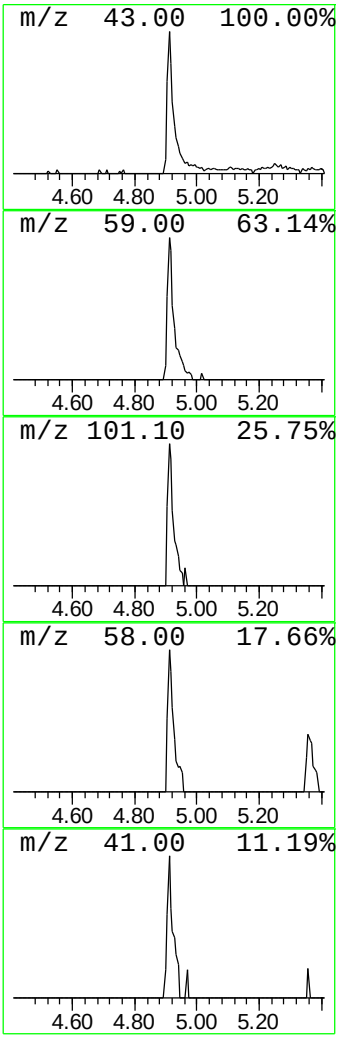
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	4.46 ng	52532	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Operator : JU
Sample : K5541-13 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 15-70-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

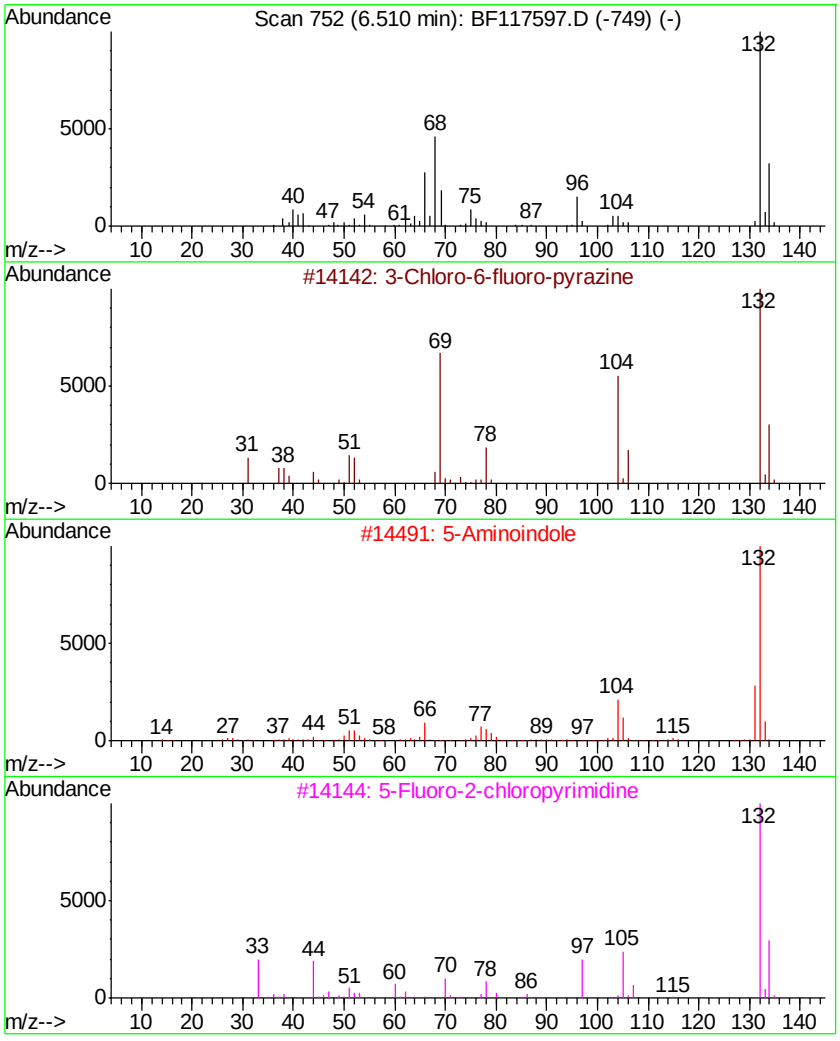
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

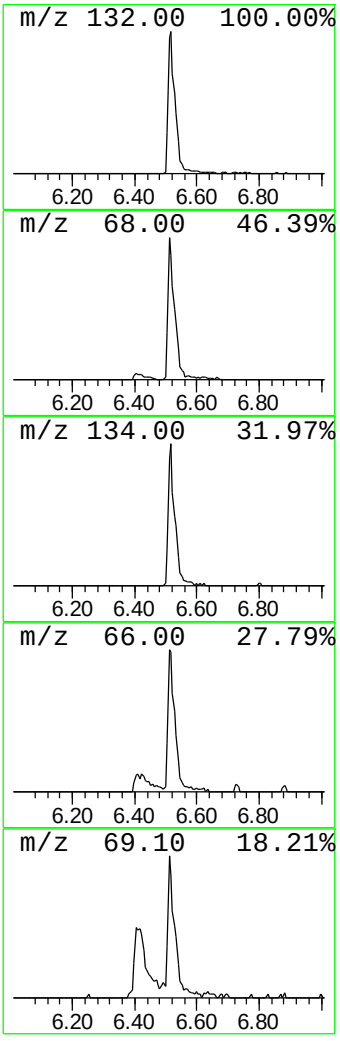
****

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	31.97 ng	376521	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Instrument : BNA_F
ClientSampleId : 15-70-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

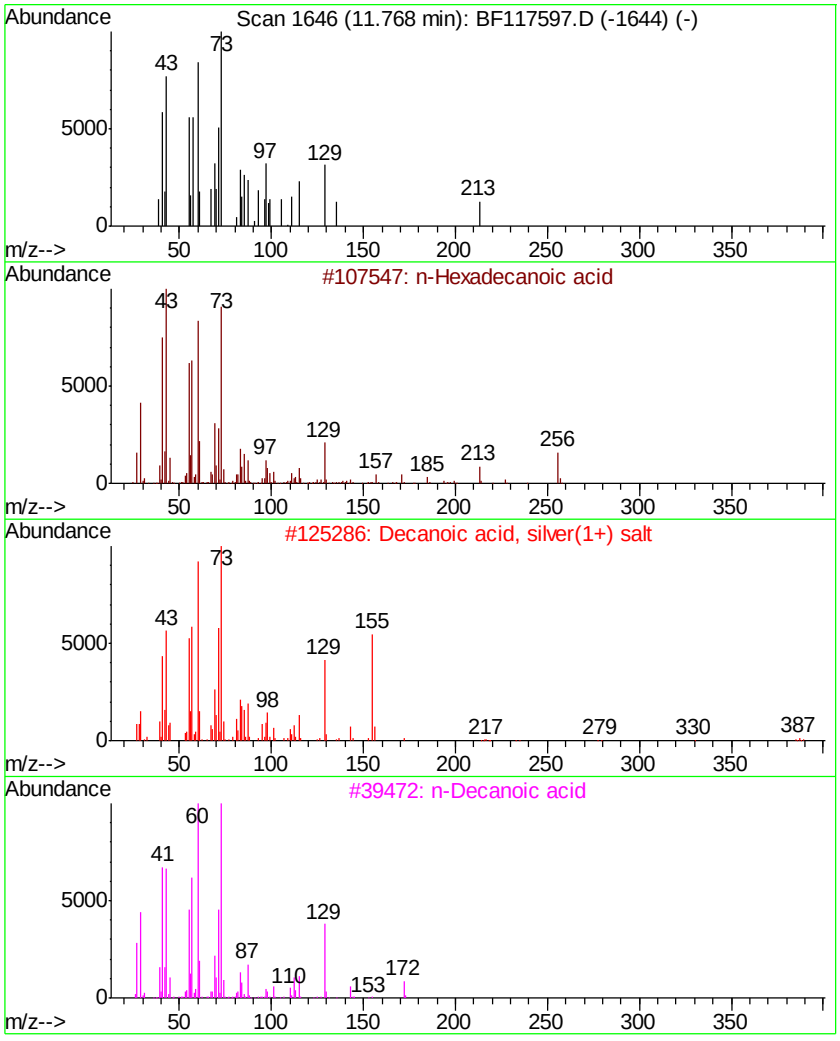
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

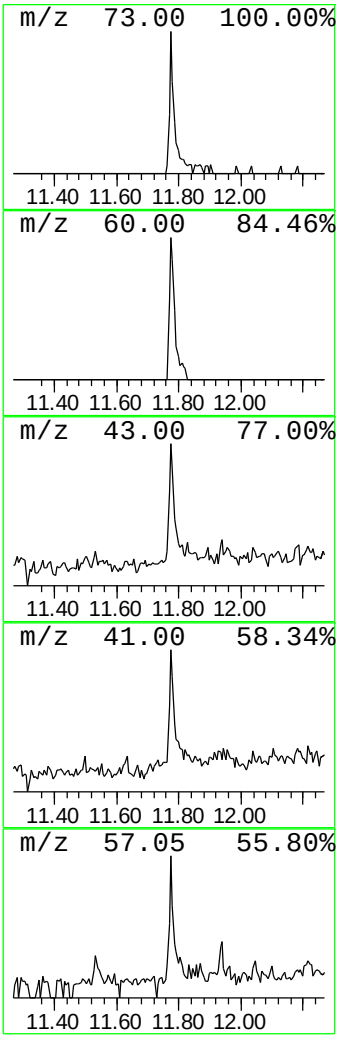
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	5.43 ng	63447	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	Tridecanoic acid	214	C13H26O2	000638-53-9	47
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	46





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 15-70-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

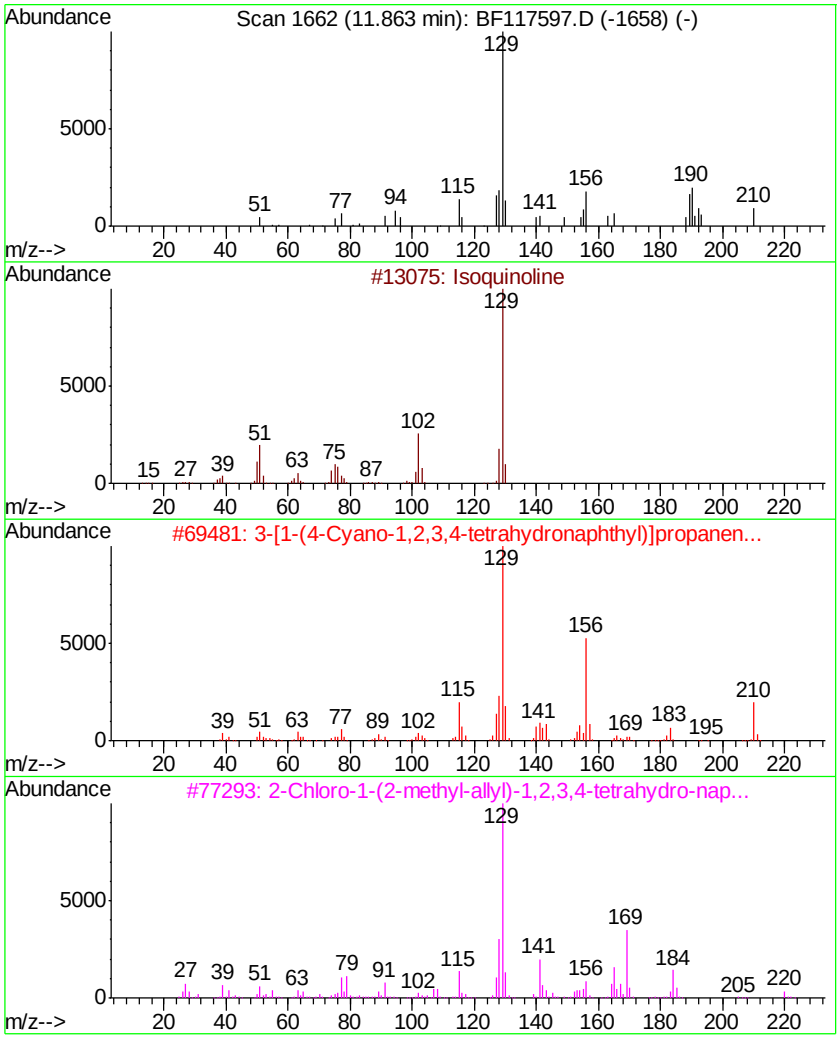
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

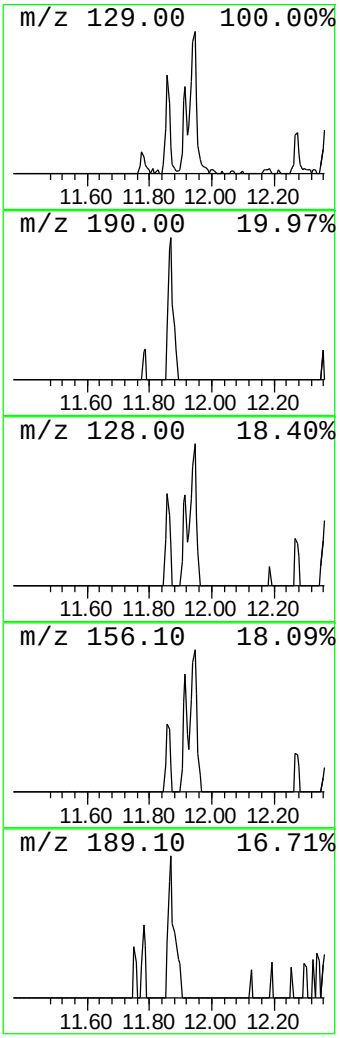
****

Peak Number 5 Isoquinoline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.66 ng	31066	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoquinoline	129	C9H7N	000119-65-3	53
2	3-[1-(4-Cyano-1,2,3,4-tetrahydro...	210	C14H14N2	057964-40-6	45
3	2-Chloro-1-(2-methyl-allyl)-1,2,...	220	C14H17Cl	1000185-82-6	45
4	Benzeneacetic acid, .alpha.-cyan...	228	C13H12N2O2	134882-04-5	42
5	1-butyne, 4-chloro-3-methyl-3-ph...	178	C11H11Cl	1000161-45-9	40





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Instrument : BNA_F
ClientSampleId : 15-70-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

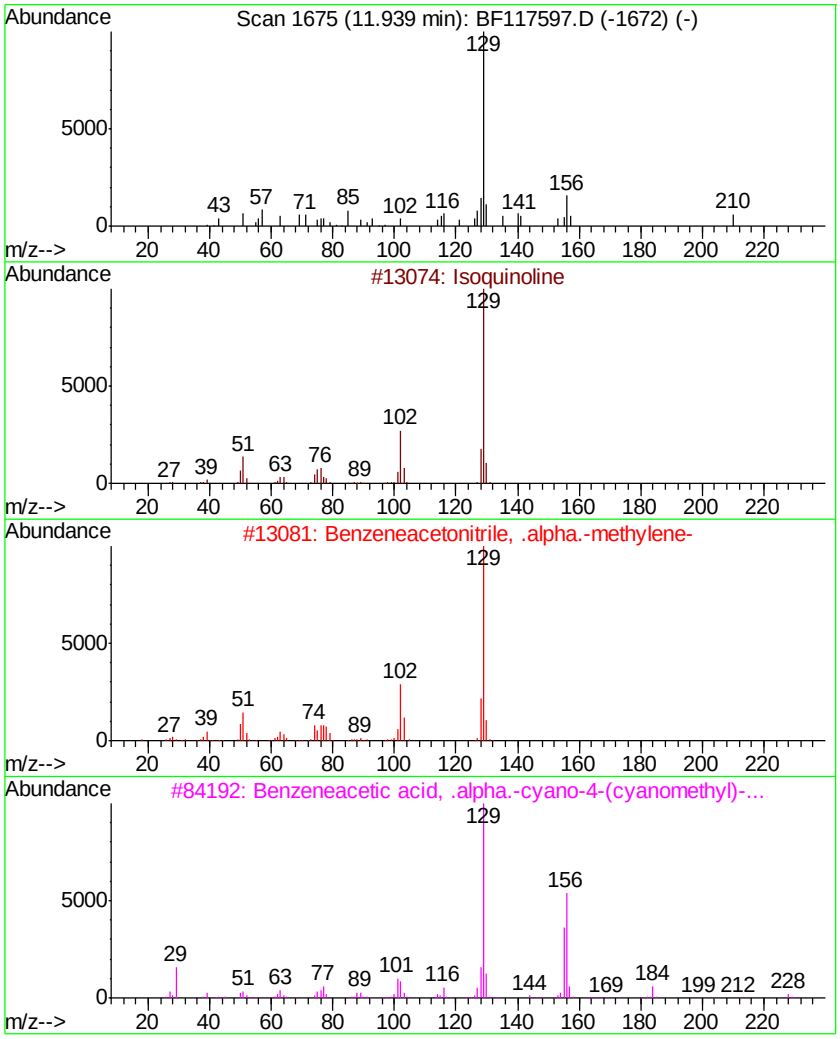
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

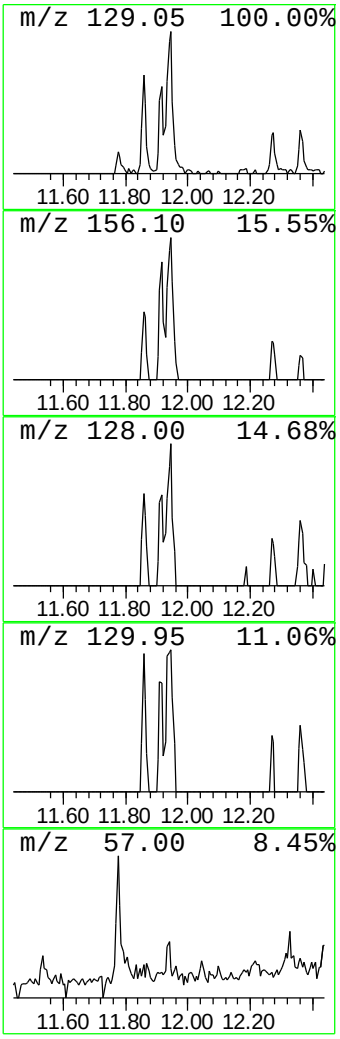
****

Peak Number 6 Benzeneacetonitrile, .alpha... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	3.95 ng	46170	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoquinoline	129	C9H7N	000119-65-3	58
2	Benzeneacetonitrile, .alpha.-met...	129	C9H7N	000495-10-3	58
3	Benzeneacetic acid, .alpha.-cyan...	228	C13H12N2O2	134882-04-5	50
4	Cyclohexanecarboxylic acid, dode...	296	C19H36O2	094107-45-6	45
5	Succinic acid, 2-decyl ethyl ester	286	C16H30O4	1000349-42-1	45





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Misc :
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Instrument : BNA_F
ClientSampleId : 15-70-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

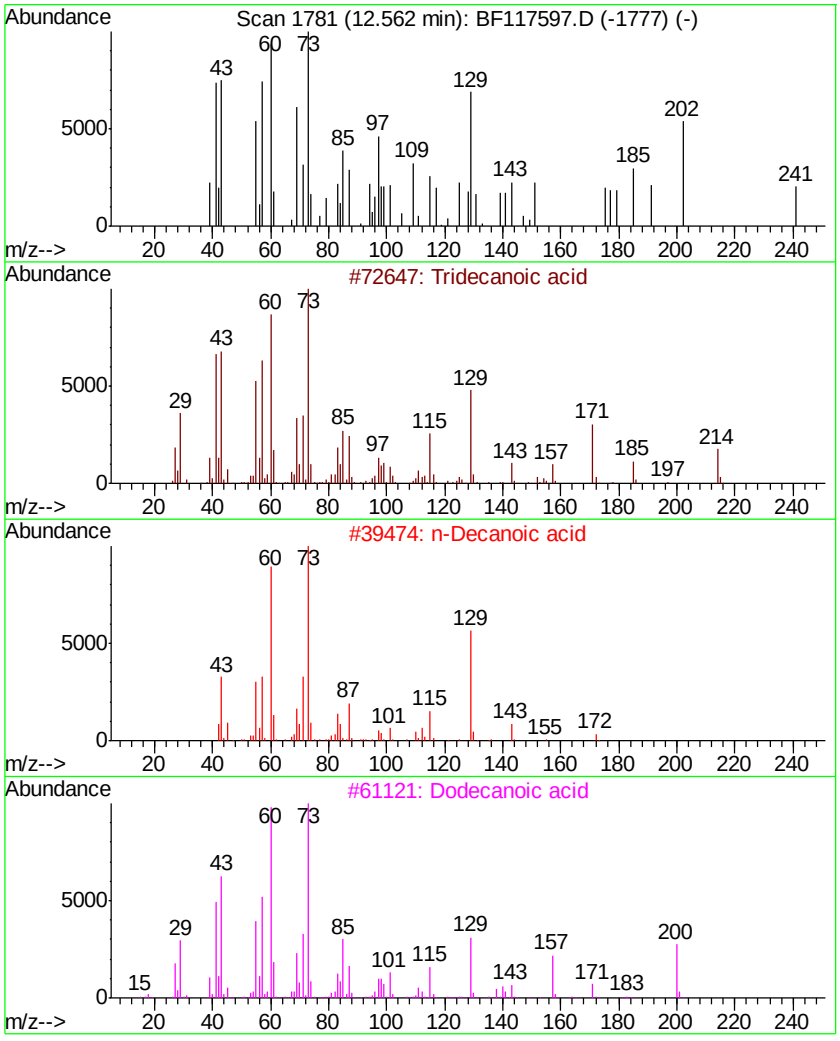
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

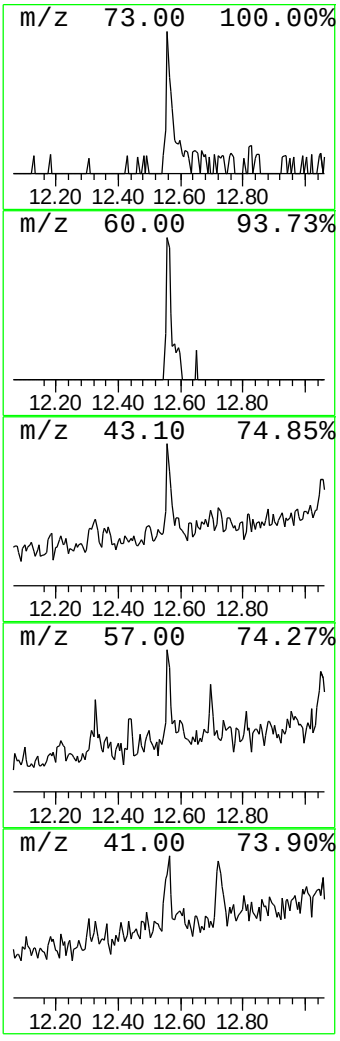
****

Peak Number 7 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	2.99 ng	34897	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	58
2	n-Decanoic acid	172	C10H20O2	000334-48-5	43
3	Dodecanoic acid	200	C12H24O2	000143-07-7	43
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	42
5	Undecanoic acid	186	C11H22O2	000112-37-8	38





Library Search Compound Report

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 15-70-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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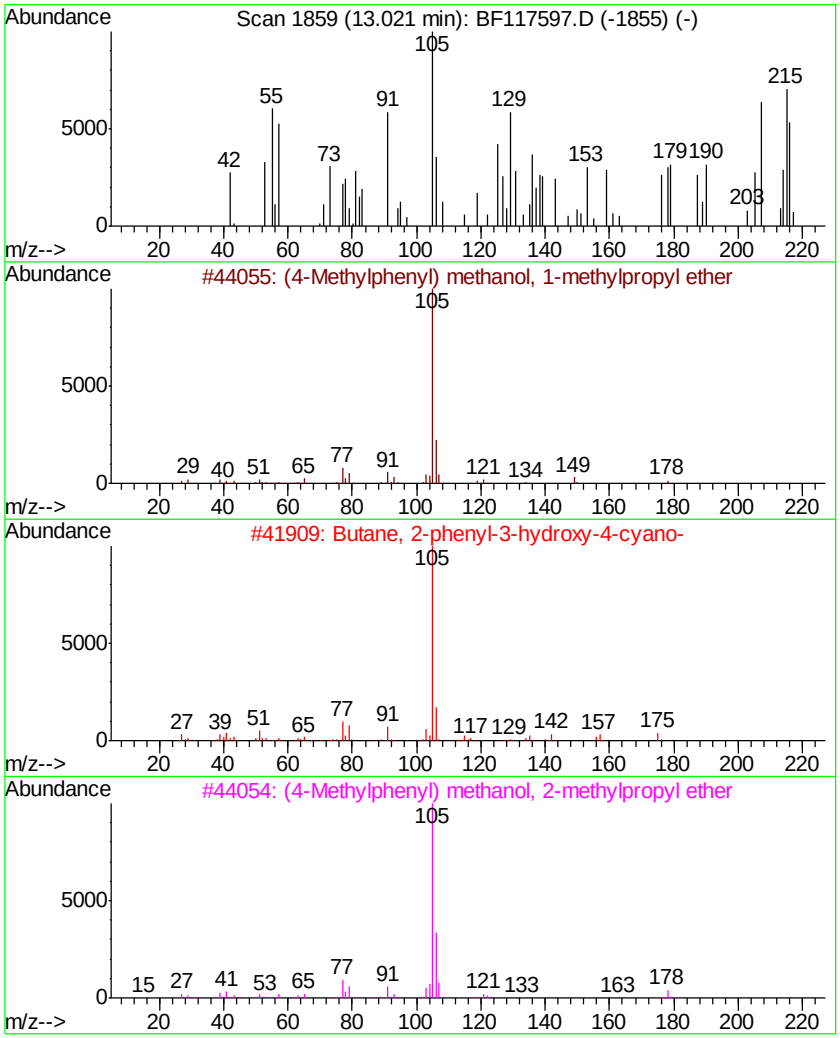
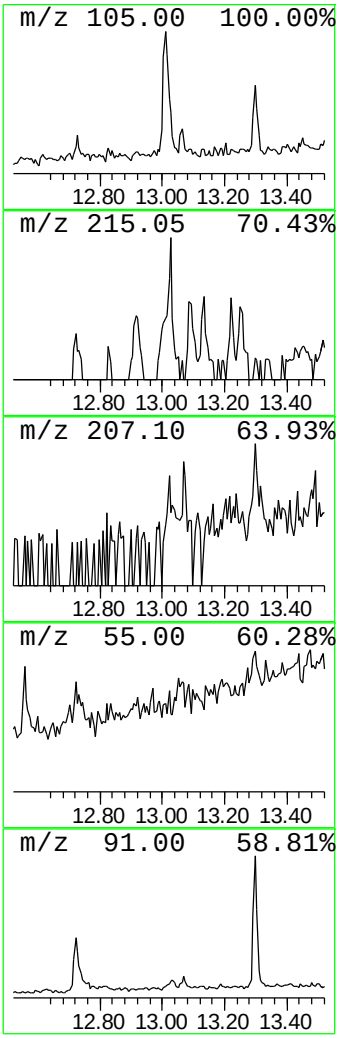
Peak Number 8 unknown13.02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.02	2.31 ng	32338	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4-Methylphenyl) methanol, 1-met...	178	C12H18O	1000374-65-6	9
2	Butane, 2-phenyl-3-hydroxy-4-cyano-	175	C11H13NO	1000162-09-2	9
3	(4-Methylphenyl) methanol, 2-met...	178	C12H18O	1000374-65-2	9
4	Benzene, (1,2-dimethyl-3-butenyl)-	160	C12H16	050871-04-0	9
5	8-Nitro-2-phenylisoxazolizidine	236	C11H12N2O4	010313-22-1	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
Data File : BF117597.D
Acq On : 29 Oct 2019 18:04
Operator : JU
Sample : K5541-13 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 15-70-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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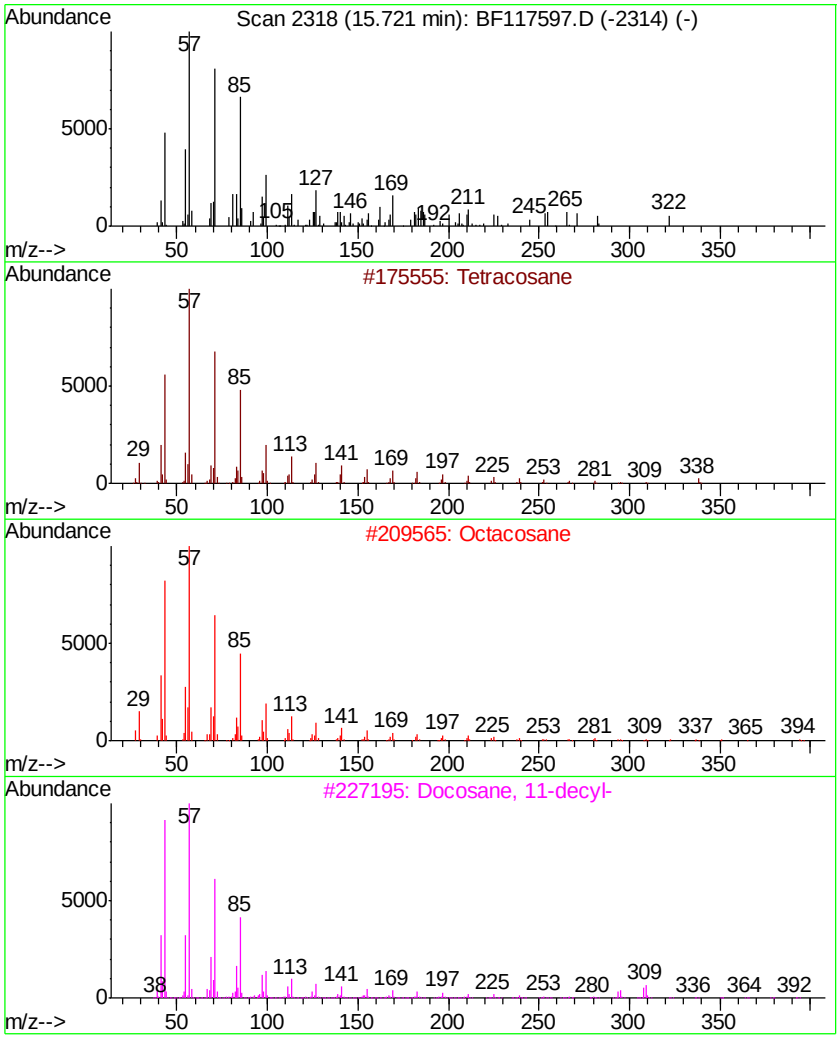
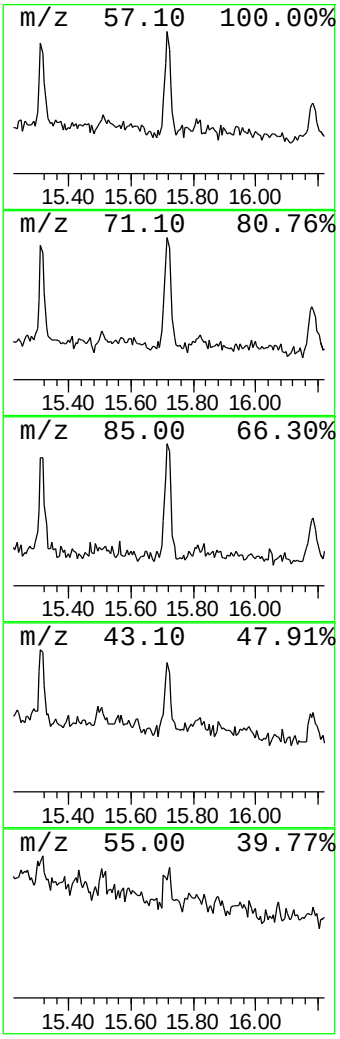
Peak Number 9 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	5.67 ng	66167	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	72
2	Octacosane	394	C28H58	000630-02-4	72
3	Docosane, 11-decyl-	451	C32H66	055401-55-3	72
4	Hexacosane	366	C26H54	000630-01-3	72
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102919\
Data File : BF117597.D
Acq On : 29 Oct 2019 18:04
Operator : JU
Sample : K5541-13 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
15-70-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
2-Pentanone, 4-hy...	4.91	4.5	ng	52532	1	6.73	235523	20.0
unknown6.51	6.51	32.0	ng	376521	1	6.73	235523	20.0
n-Hexadecanoic acid	11.77	5.4	ng	63447	4	11.24	233725	20.0
Isoquinoline	11.86	2.7	ng	31066	4	11.24	233725	20.0
Benzeneacetonitri...	11.94	4.0	ng	46170	4	11.24	233725	20.0
Tridecanoic acid	12.56	3.0	ng	34897	4	11.24	233725	20.0
unknown13.02	13.02	2.3	ng	32338	5	13.89	279550	20.0
Tetracosane	15.72	5.7	ng	66167	6	15.33	233192	20.0