LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097965.D
Acq On : 22 Aug 2017 20:38
Operator : SJ/JU
Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-TP-106-E(0-5)COMP

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-BF081517.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	4.934	481	484	492	rVB	135929	166495	6.44%	0.688%
2	5.351	550	555	558	rBV	2081412	1945780	75.30%	8.037%
3	6.381	724	730	741	rVB	1977319	2046510	79.20%	8.453%
4	6.516	748	753	756	rBV	2100147	1994308	77.18%	8.238%
5	6.745	788	792	796	rBV	1081232	902728	34.93%	3.729%
6	6.904	814	819	822	rBV	2033693	1842004	71.28%	7.609%
7	7.310	883	888	891	rBV	1675183	1556530	60.24%	6.429%
8	8.028	1006	1010	1014	rBV	1370179	1183016	45.78%	4.887%
9	9.110	1188	1194	1197	rBV	2543734	2584084	100.00%	10.674%
10	9.498	1257	1260	1265	rBV	217840	176135	6.82%	0.728%
11	9.780	1302	1308	1312	rBV2	1341432	1210711	46.85%	5.001%
12	10.192	1375	1378	1381	rBV2	28525	36932	1.43%	0.153%
13	10.563	1437	1441	1449	rBV	1110078	1105005	42.76%	4.564%
14	10.692	1460	1463	1471	rBV2	42297	55965	2.17%	0.231%
15	11.139	1536	1539	1542	rBV	32849	28170	1.09%	0.116%
16	11.263	1556	1560	1563	rBV	1287365	1084452	41.97%	4.479%
17	11.286	1563	1564	1567	rVV	92617	44778	1.73%	0.185%
18	11.333	1567	1572	1575	rVB	35629	37874	1.47%	0.156%
19	11.869	1660	1663	1666	rBV2	26081	30700	1.19%	0.127%
20	11.969	1678	1680	1683	rBV2	30613	29518	1.14%	0.122%
21	12.310	1735	1738	1742	rBV3	24383	26193	1.01%	0.108%
22	12.469	1761	1765	1768	rBV	195887	161941	6.27%	0.669%
23	12.674	1797	1800	1802	rBV	404555	375970	14.55%	1.553%
24	12.698	1802	1804	1807	rVV	180503	148426	5.74%	0.613%
25	12.733	1807	1810	1811	rVV2	37283	36171	1.40%	0.149%
26	12.751	1811	1813	1818	rVB2	92644	80864	3.13%	0.334%
27	12.845	1825	1829	1833	rBV	1705176	1714143	66.33%	7.081%
28	12.916	1837	1841	1844	rBV3	20846	32947	1.27%	0.136%
29	13.027	1858	1860	1864	rVB	39321	32583	1.26%	0.135%
30	13.086	1868	1870	1873	rVB2	44449	39734	1.54%	0.164%
31	13.127	1874	1877	1882	rBV2	36046	42861	1.66%	0.177%
32	13.221	1890	1893	1896	rVB	32012	26859	1.04%	0.111%
33	13.380	1917	1920	1923	rBV	266217	230592	8.92%	0.952%
34	13.427	1923	1928	1930	rVV2	64705	81238	3.14%	0.336%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-TP-106-E(0-5)COMP

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.757	1980	1984	1991	rVB3	78769	114166	4.42%	0.472%
36	13.892	2003	2007	2010	rBV	861119	943118	36.50%	3.896%
37	13.916	2010	2011	2014	rVB	92160	67697	2.62%	0.280%
38	14.074	2035	2038	2041	rBV2	75366	67785	2.62%	0.280%
39	14.374	2087	2089	2092	rBV	69591	66495	2.57%	0.275%
40	14.674	2138	2140	2143	rVB	55405	41679	1.61%	0.172%
41	14.910	2176	2180	2188	rBV	147701	275436	10.66%	1.138%
42	14.998	2193	2195	2201	rVB2	71821	104227	4.03%	0.431%
43	15.192	2225	2228	2234	rVB	107760	135027	5.23%	0.558%
44	15.257	2235	2239	2242	rBV	128606	170594	6.60%	0.705%
45	15.315	2245	2249	2253	rBV	579030	720262	27.87%	2.975%
46	15.774	2324	2327	2331	rBV3	53319	82008	3.17%	0.339%
47	15.986	2360	2363	2373	rVB2	92585	182405	7.06%	0.753%
48	16.398	2430	2433	2442	rVB3	77051	146222	5.66%	0.604%

Sum of corrected areas: 24209338

LSC Report - Integrated Chromatogram

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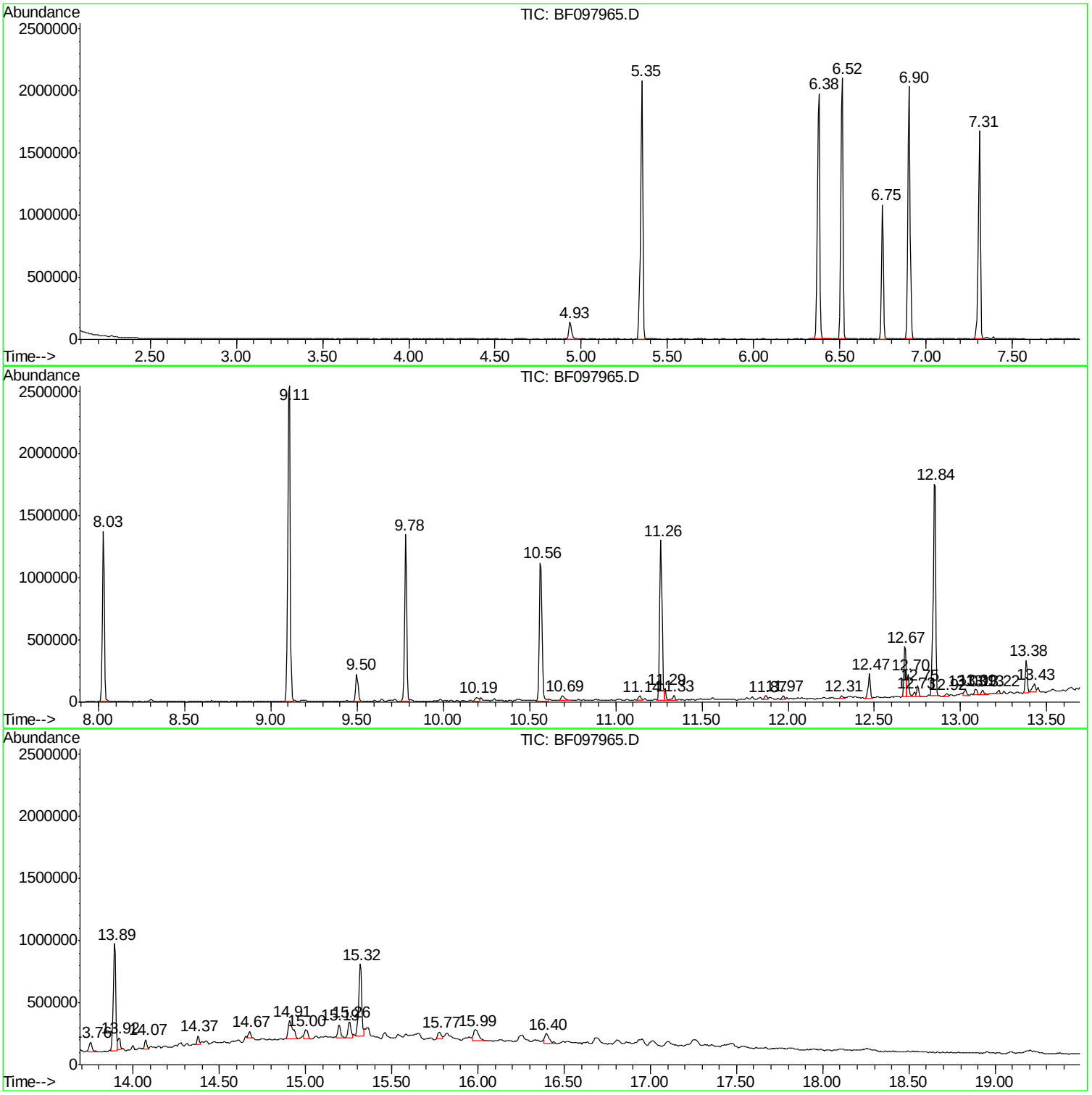
Operator : SJ/JU
Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-E(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097965.D
Acq On : 22 Aug 2017 20:38
Operator : SJ/JU
Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-E(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

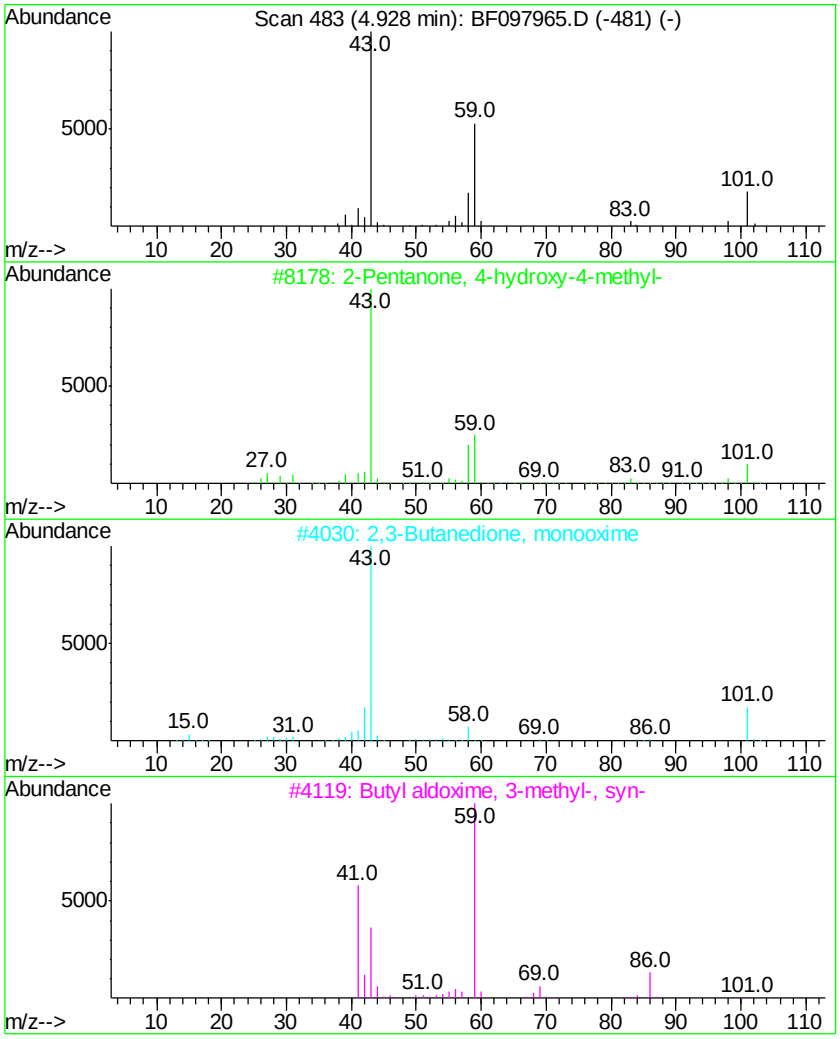
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

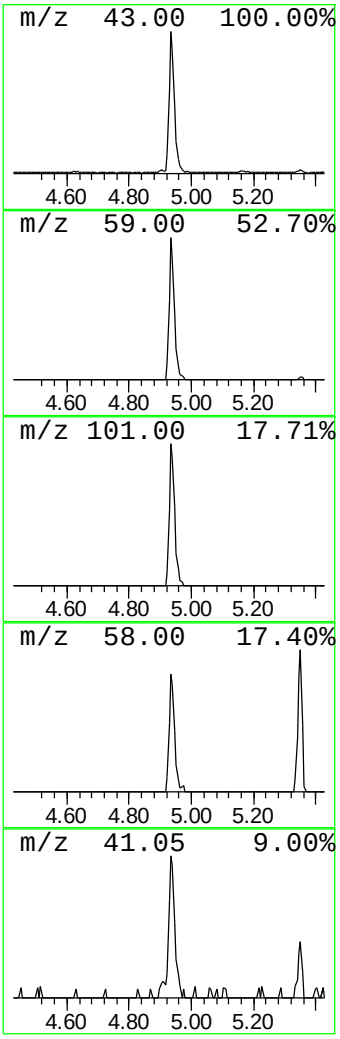
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	3.69 ng	166495	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Acetone	58	C3H6O	000067-64-1	9





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Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-E(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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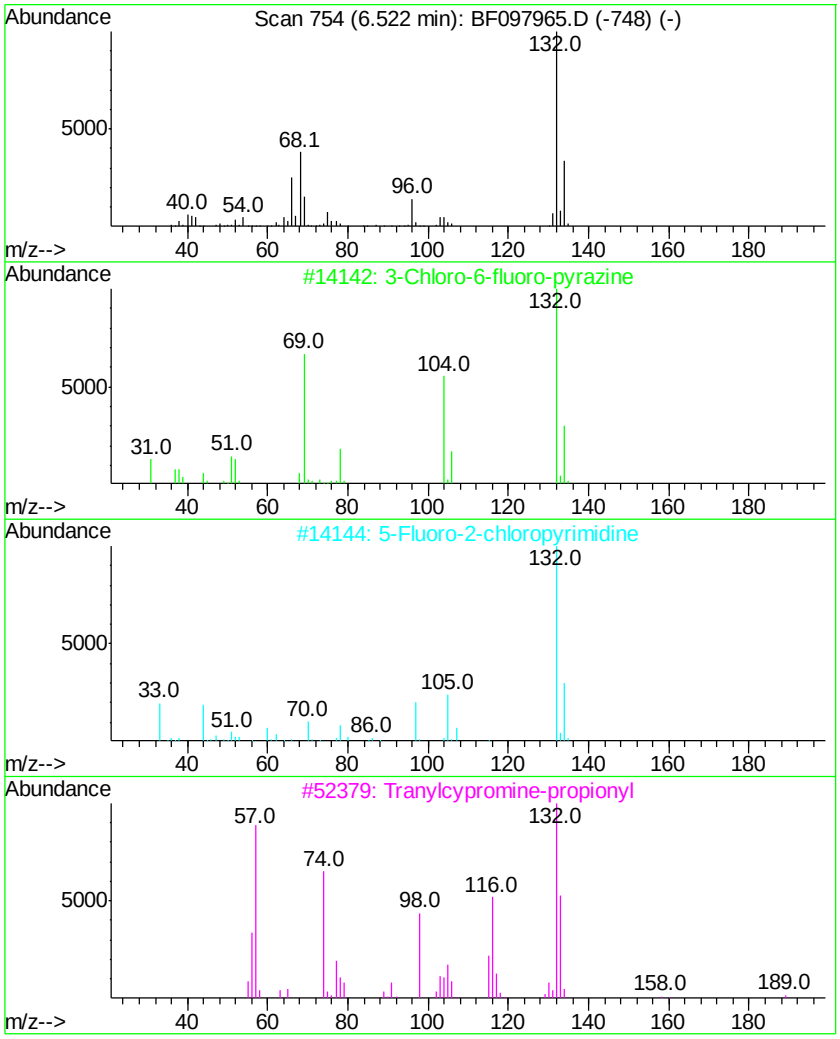
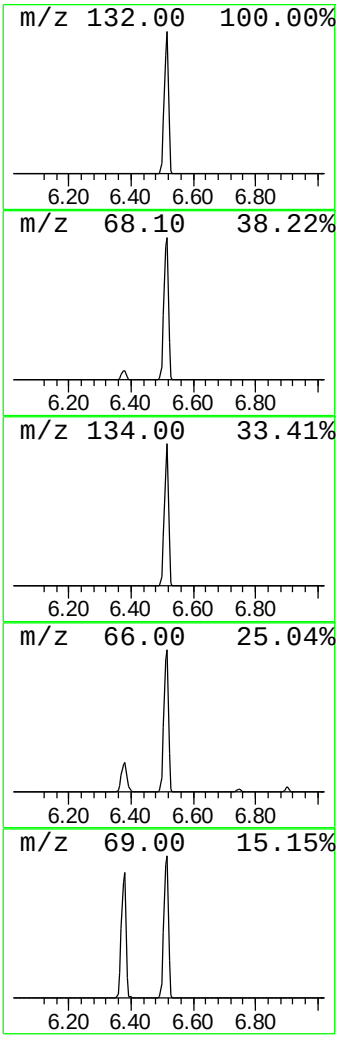
Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	44.18 ng	1994310	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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





Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097965.D
Acq On : 22 Aug 2017 20:38
Operator : SJ/JU
Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-E(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

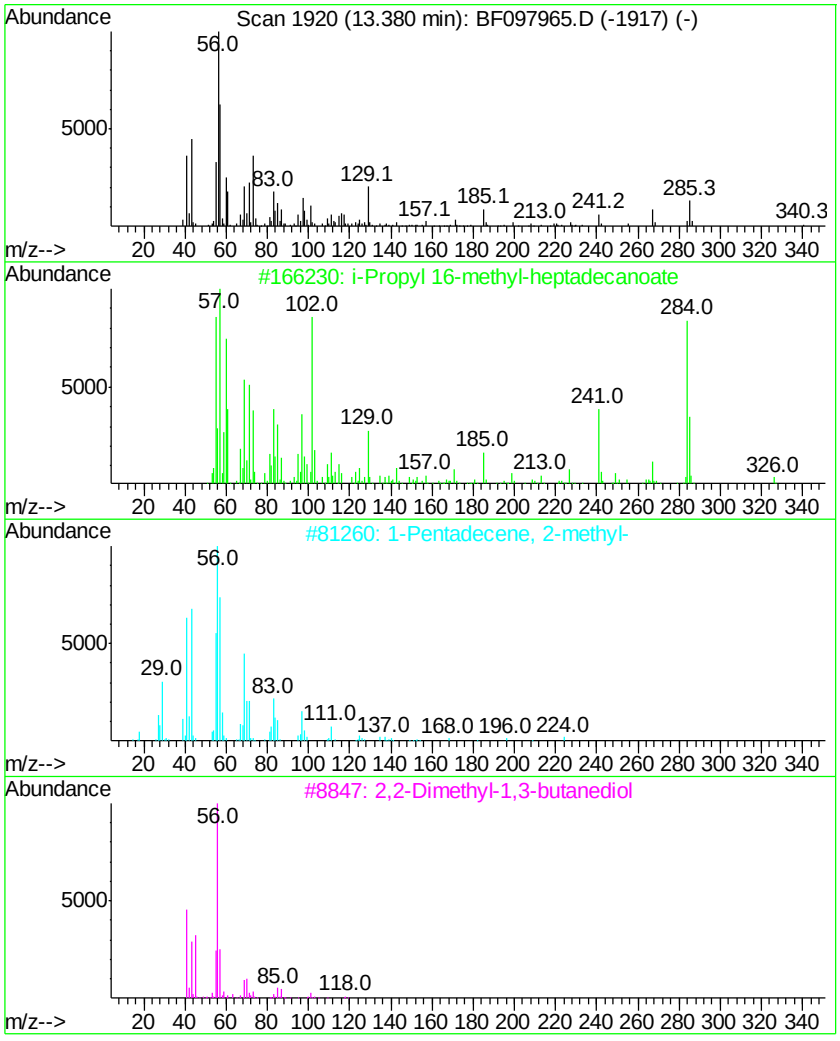
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

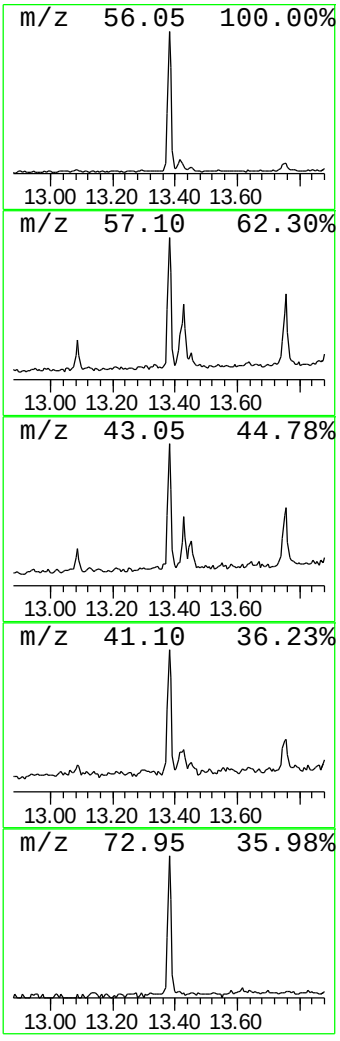
****

Peak Number 4 unknown13.38 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	4.89 ng	230592	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	i-Propyl 16-methyl-heptadecanoate	326	C21H42O2	1000336-66-3	38
2	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37
3	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	35
4	2-Methyl-1-octadecene	266	C19H38	061868-20-0	35
5	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35





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Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-E(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

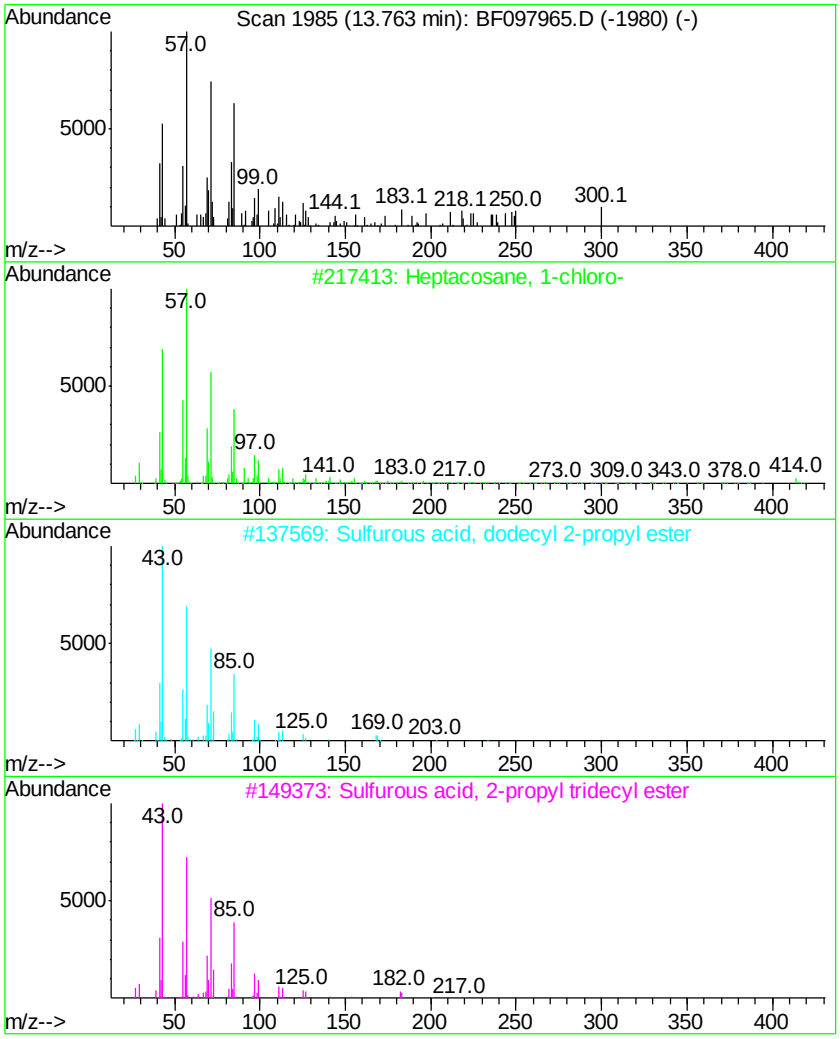
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

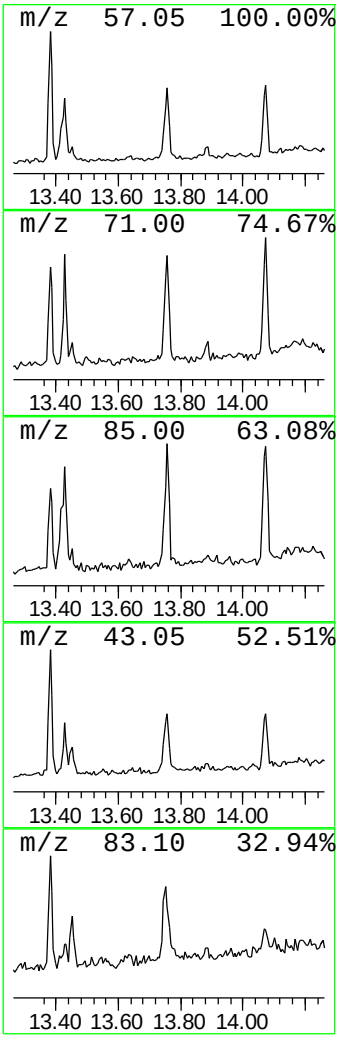
****

Peak Number 5 Heptacosane, 1-chloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	2.42 ng	114166	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
2	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	91
3	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91
4	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91
5	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	86





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Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-E(0-5)COMP

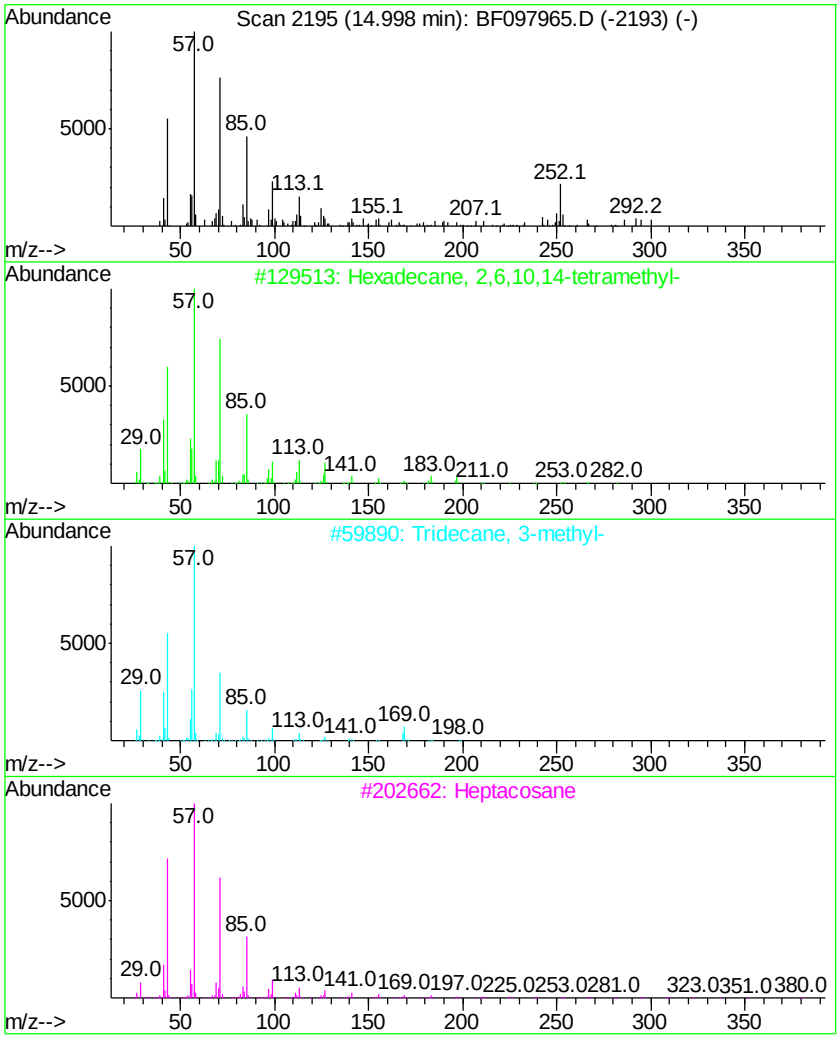
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

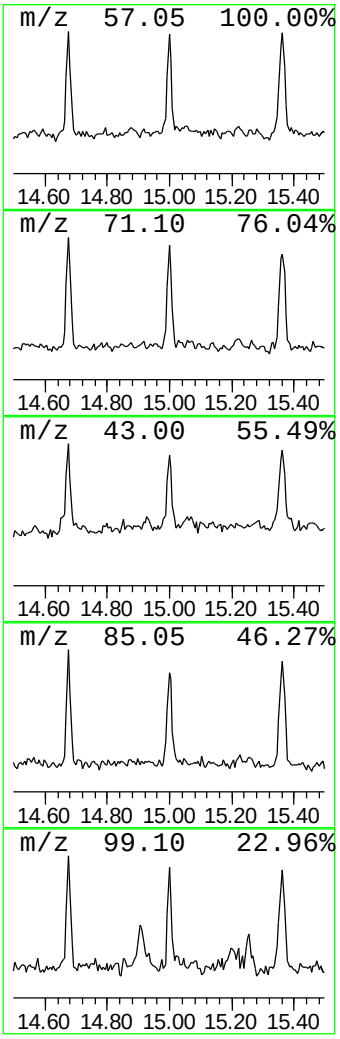
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.89 ng	104227	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	58
3	Heptacosane	380	C27H56	000593-49-7	52
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	50
5	Tridecane	184	C13H28	000629-50-5	50





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Sample : I4889-03
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

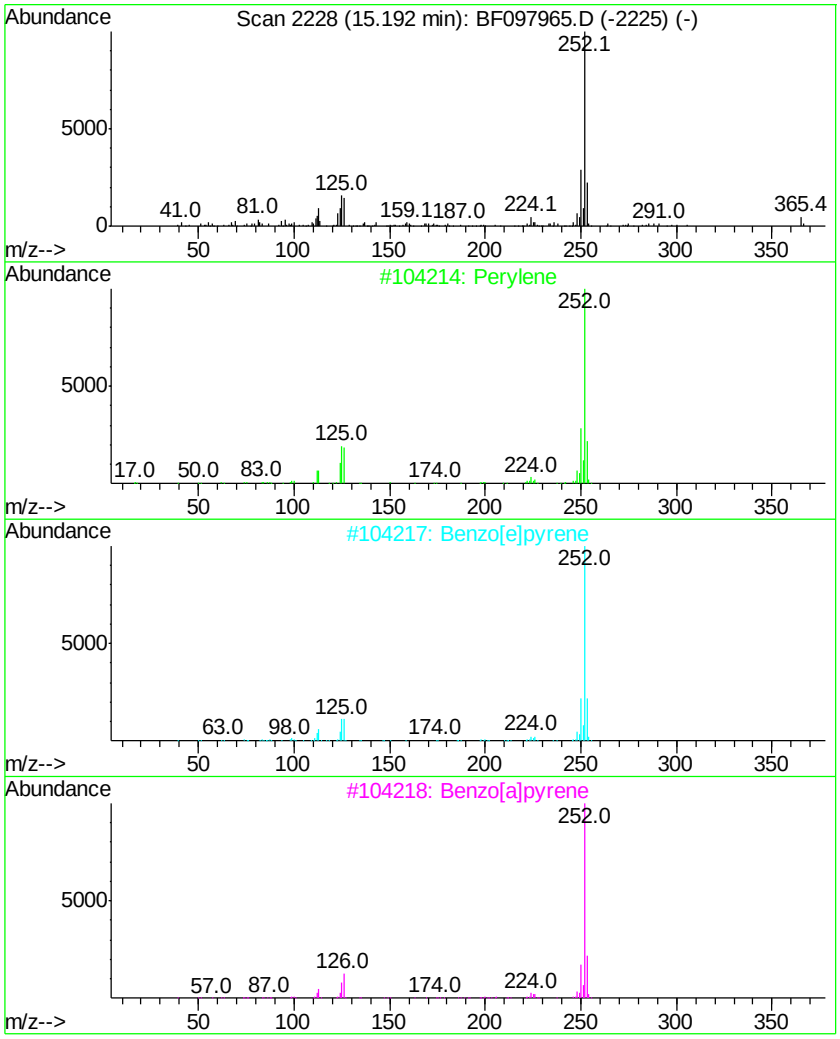
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

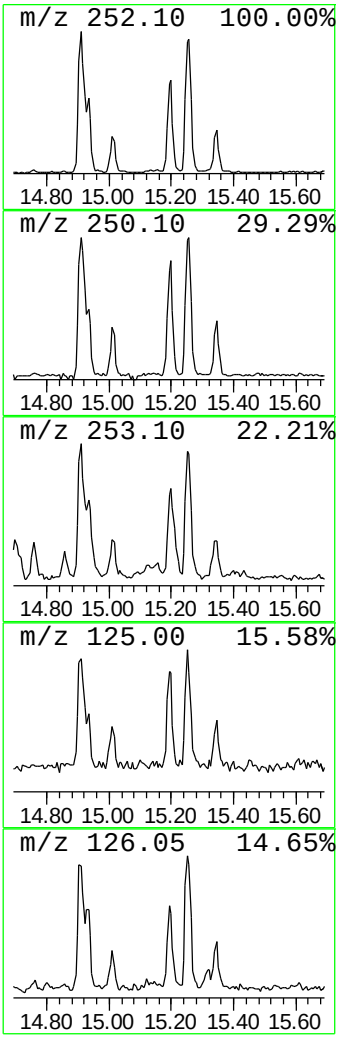
****

Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	3.75 ng	135027	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	93
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097965.D
Acq On : 22 Aug 2017 20:38
Operator : SJ/JU
Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-E(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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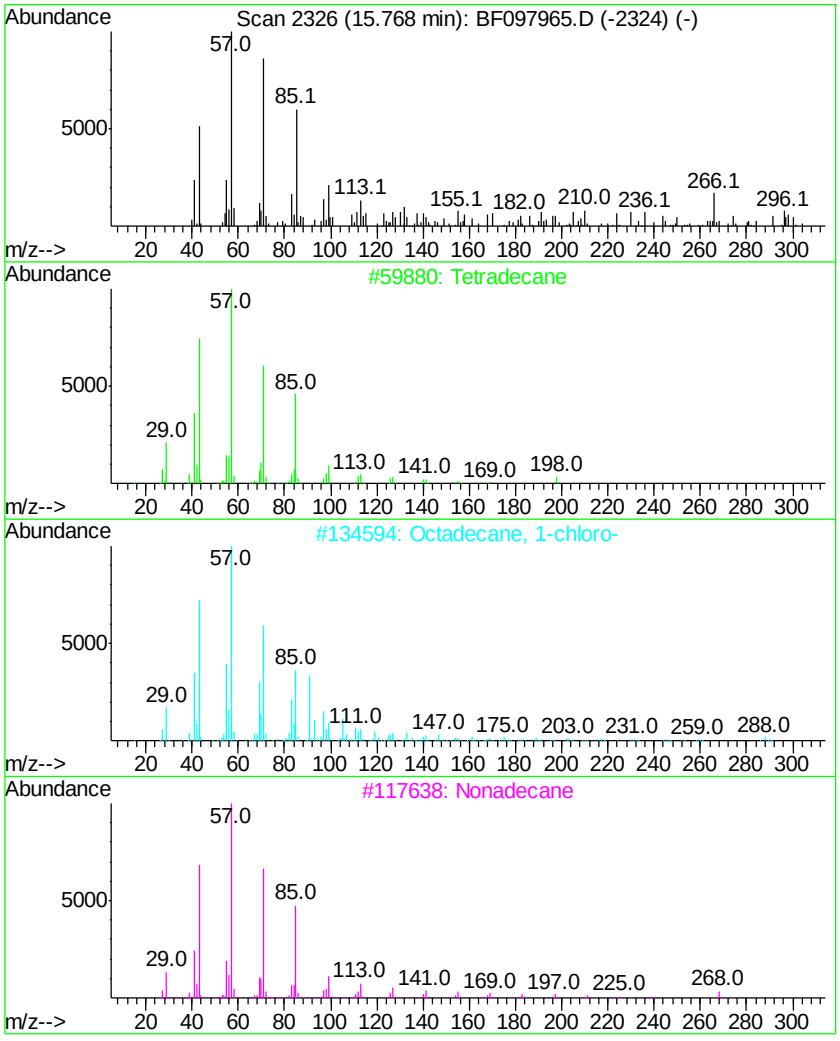
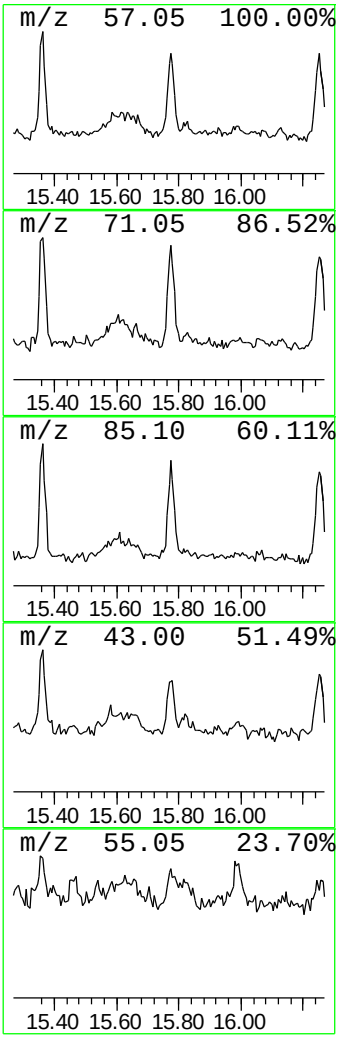
Peak Number 8 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.28 ng	82008	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	64
2	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	64
3	Nonadecane	268	C19H40	000629-92-5	62
4	Octacosane	394	C28H58	000630-02-4	58
5	Docosane	310	C22H46	000629-97-0	58





Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
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Operator : SJ/JU
Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-TP-106-E(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

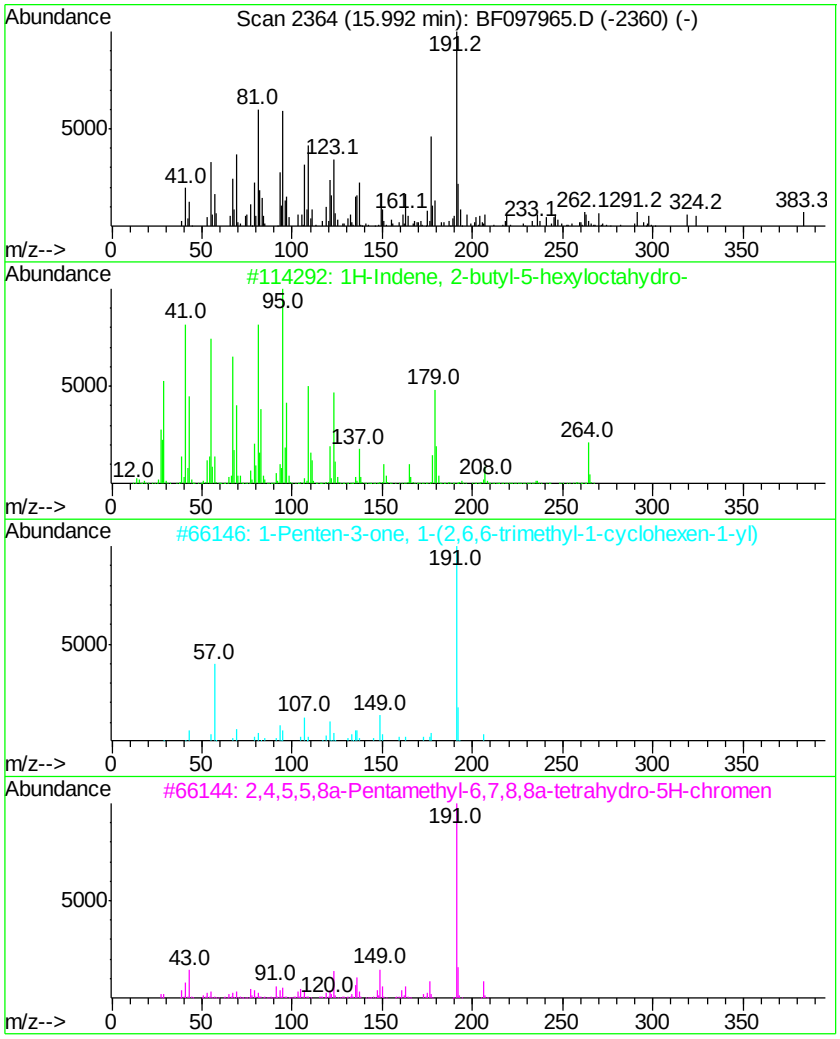
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

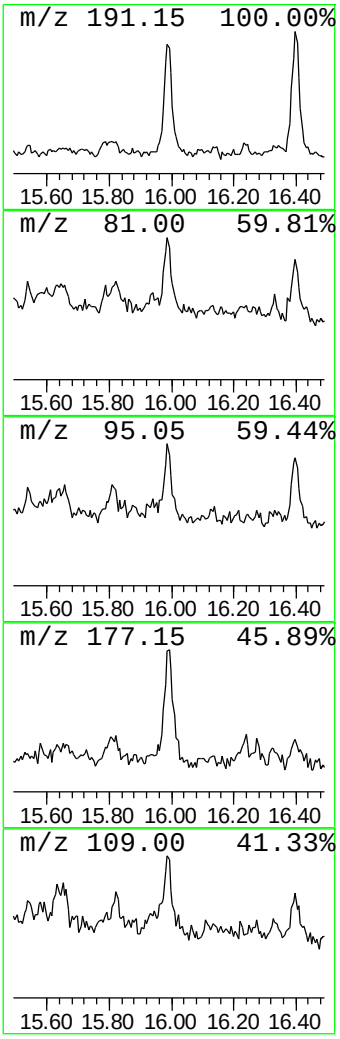
****

Peak Number 9 1H-Indene, 2-butyl-5-hexylo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	5.06 ng	182405	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2-butyl-5-hexyloctahy...	264	C19H36	055044-33-2	55
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	27
3	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	27
4	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	25
5	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	25





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097965.D
Acq On : 22 Aug 2017 20:38
Operator : SJ/JU
Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-E(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

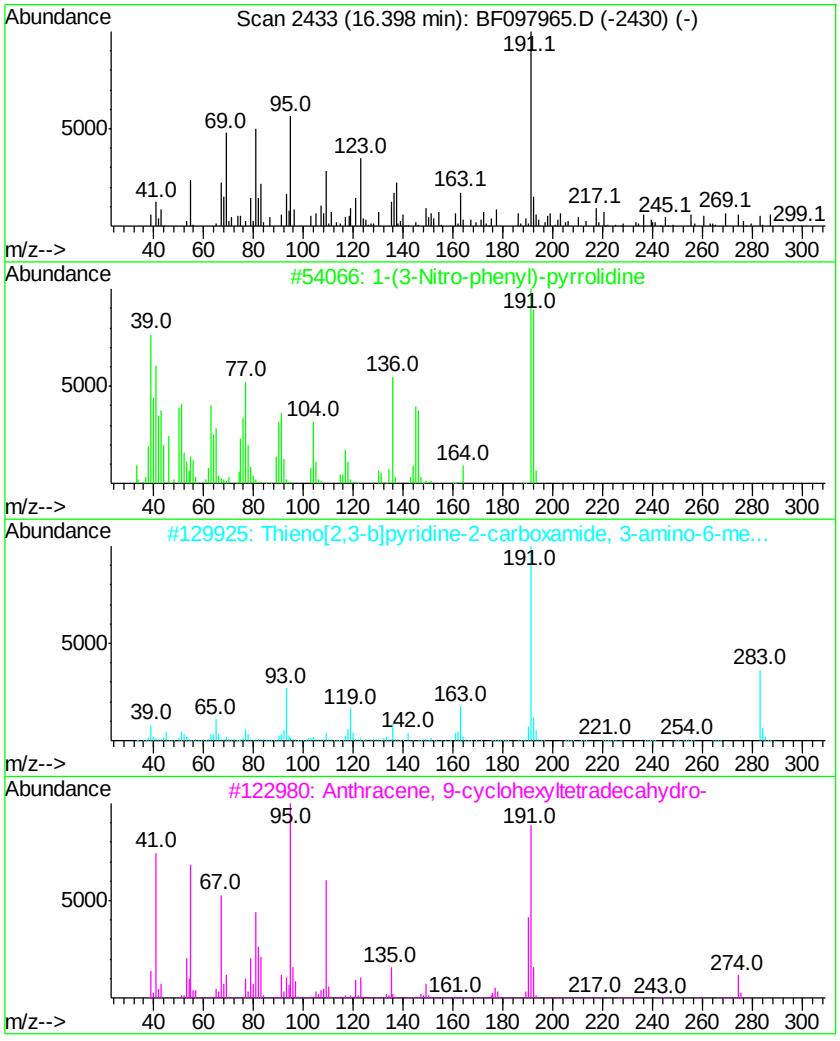
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

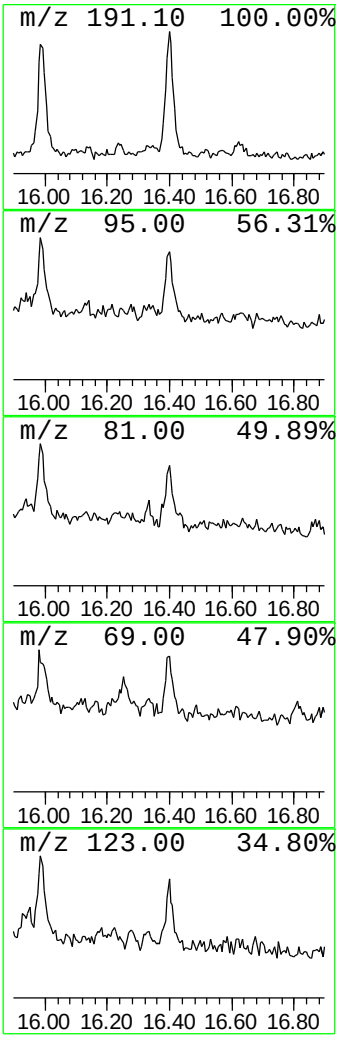
****

Peak Number 10 unknown16.40 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	4.06 ng	146222	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(3-Nitro-phenyl)-pyrrolidine	192	C10H12N2O2	1000300-34-7	42
2	Thieno[2,3-b]pyridine-2-carboxam...	283	C15H13N3OS	1000350-91-6	41
3	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	38
4	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	38
5	9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	38





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF082217\
Data File : BF097965.D
Acq On : 22 Aug 2017 20:38
Operator : SJ/JU
Sample : I4889-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-TP-106-E(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.93	3.7	ng	166495	1	6.75	902728	20.0
unknown6.52	6.52	44.2	ng	1994310	1	6.75	902728	20.0
unknown13.38	13.38	4.9	ng	230592	5	13.90	943118	20.0
Heptacosane, 1-ch...	13.76	2.4	ng	114166	5	13.90	943118	20.0
Hexadecane, 2,6,1...	15.00	2.9	ng	104227	6	15.32	720262	20.0
Perylene	15.19	3.8	ng	135027	6	15.32	720262	20.0
Tetradecane	15.77	2.3	ng	82008	6	15.32	720262	20.0
1H-Indene, 2-buty...	15.99	5.1	ng	182405	6	15.32	720262	20.0
unknown16.40	16.40	4.1	ng	146222	6	15.32	720262	20.0