LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
Data File : BN000837.D
Acq On : 23 Apr 2018 21:01
Operator : JU/SJ
Sample : J2467-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : A3XZ9

Integration Parameters: events.e
Integrator: ChemStation
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_N\METHODS\SOM-EPA-BN041918-PAH.M
Title : ??? S

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.799	642	648	660	rVB	175627	281552	9.16%	0.833%
2	6.969	670	677	689	rBV	650838	967457	31.49%	2.862%
3	7.158	703	709	716	rBV	635133	958467	31.20%	2.835%
4	7.622	781	788	796	rVB	627766	946753	30.82%	2.801%
5	8.322	900	907	918	rBV	501966	775756	25.25%	2.295%
6	8.764	974	982	991	rBV	724272	1112638	36.22%	3.291%
7	9.475	1096	1103	1111	rBV	566225	903213	29.40%	2.672%
8	10.011	1187	1194	1207	rBV	861995	1376406	44.80%	4.072%
9	10.387	1251	1258	1265	rBV	861843	1408424	45.85%	4.166%
10	13.669	1810	1816	1820	rBV	1500964	1982539	64.53%	5.865%
11	13.716	1820	1824	1829	rVB	204034	270277	8.80%	0.800%
12	13.940	1855	1862	1874	rBV	1735879	2534687	82.51%	7.498%
13	14.175	1897	1902	1907	rBV	47509	60662	1.97%	0.179%
14	14.251	1908	1915	1923	rBV2	1160015	1755937	57.16%	5.194%
15	14.451	1943	1949	1958	rBV	89914	136006	4.43%	0.402%
16	15.134	2060	2065	2070	rVB	57932	70325	2.29%	0.208%
17	15.251	2078	2085	2094	rVB	2016594	2964047	96.48%	8.768%
18	15.363	2099	2104	2112	rBV	635035	852887	27.76%	2.523%
19	15.993	2206	2211	2215	rBV	52431	68752	2.24%	0.203%
20	16.787	2340	2346	2350	rBV	41774	50752	1.65%	0.150%
21	16.998	2376	2382	2389	rBV2	1392533	1898634	61.80%	5.617%
22	17.098	2391	2399	2408	rBV	2078761	2930370	95.39%	8.669%
23	17.910	2532	2537	2546	rBV	82642	123134	4.01%	0.364%
24	19.028	2722	2727	2733	rBV	20208	30937	1.01%	0.092%
25	19.204	2753	2757	2766	rBV2	48594	63525	2.07%	0.188%
26	19.398	2784	2790	2805	rVB2	2304089	3072143	100.00%	9.088%
27	20.939	3049	3052	3061	rBV5	18333	37884	1.23%	0.112%
28	21.198	3091	3096	3105	rBV	1356342	1718299	55.93%	5.083%
29	22.269	3275	3278	3285	rVB	30739	38120	1.24%	0.113%
30	22.392	3296	3299	3304	rVB	30371	38727	1.26%	0.115%
31	22.763	3358	3362	3368	rVB	50153	66636	2.17%	0.197%
32	23.251	3438	3445	3452	rBV2	1356219	2433792	79.22%	7.200%
33	23.316	3452	3456	3460	rVV	60247	93542	3.04%	0.277%
34	23.386	3461	3468	3477	rVB	863869	1560265	50.79%	4.616%

LSC Area Percent Report

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Data File : BN000837.D
Acq On : 23 Apr 2018 21:01
Operator : JU/SJ
Sample : J2467-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : A3XZ9

Integration Parameters: events.e
Integrator: ChemStation
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_N\METHODS\SOM-EPA-BN041918-PAH.M
Title : ??? S

35	23.939	3558	3562	3572	rVB	60045	102450	3.33%	0.303%
36	24.663	3680	3685	3697	rVB2	54365	118377	3.85%	0.350%

Sum of corrected areas: 33804372

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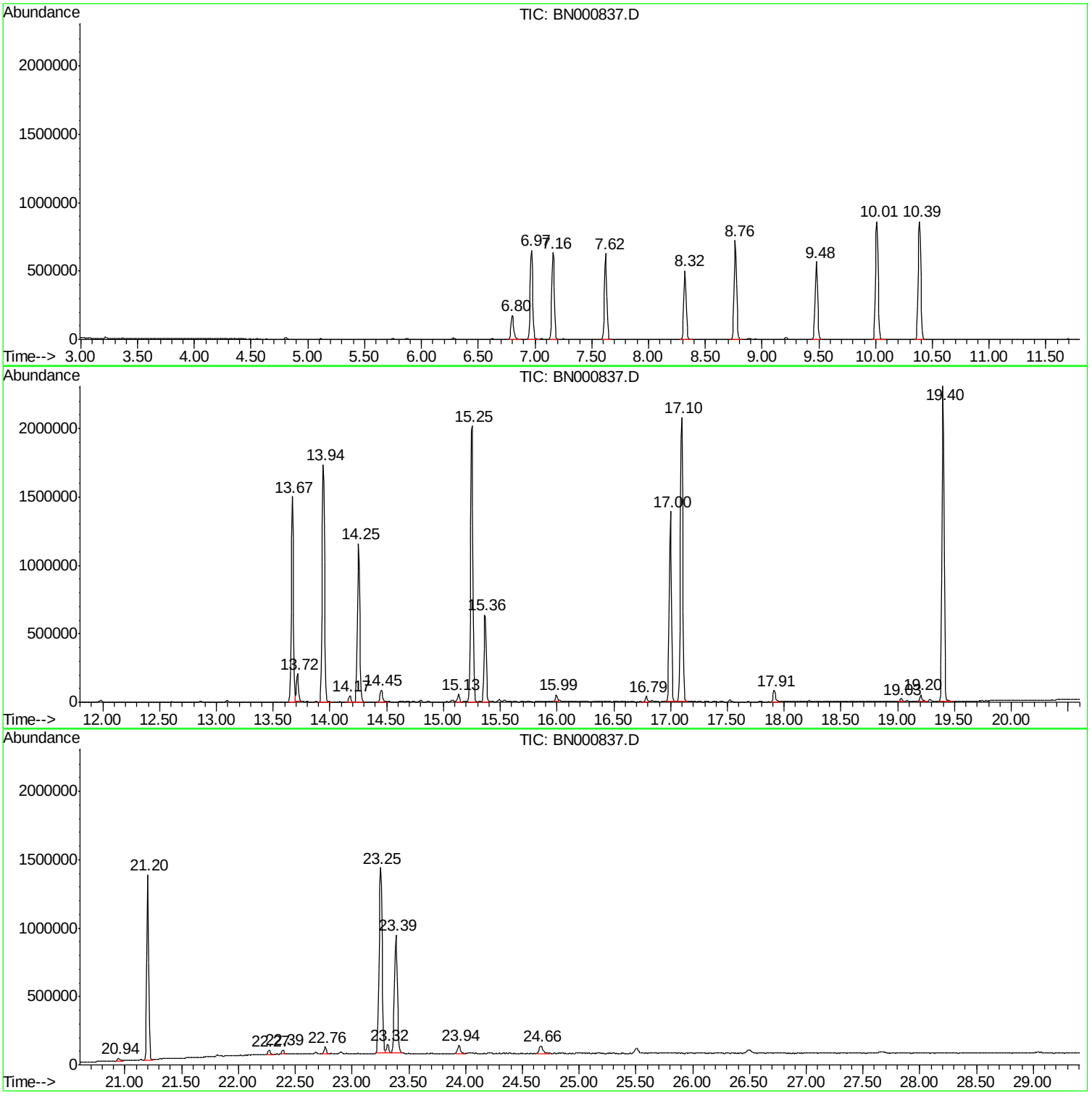
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A3XZ9

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

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



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Data File : BN000837.D
Acq On : 23 Apr 2018 21:01
Operator : JU/SJ
Sample : J2467-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

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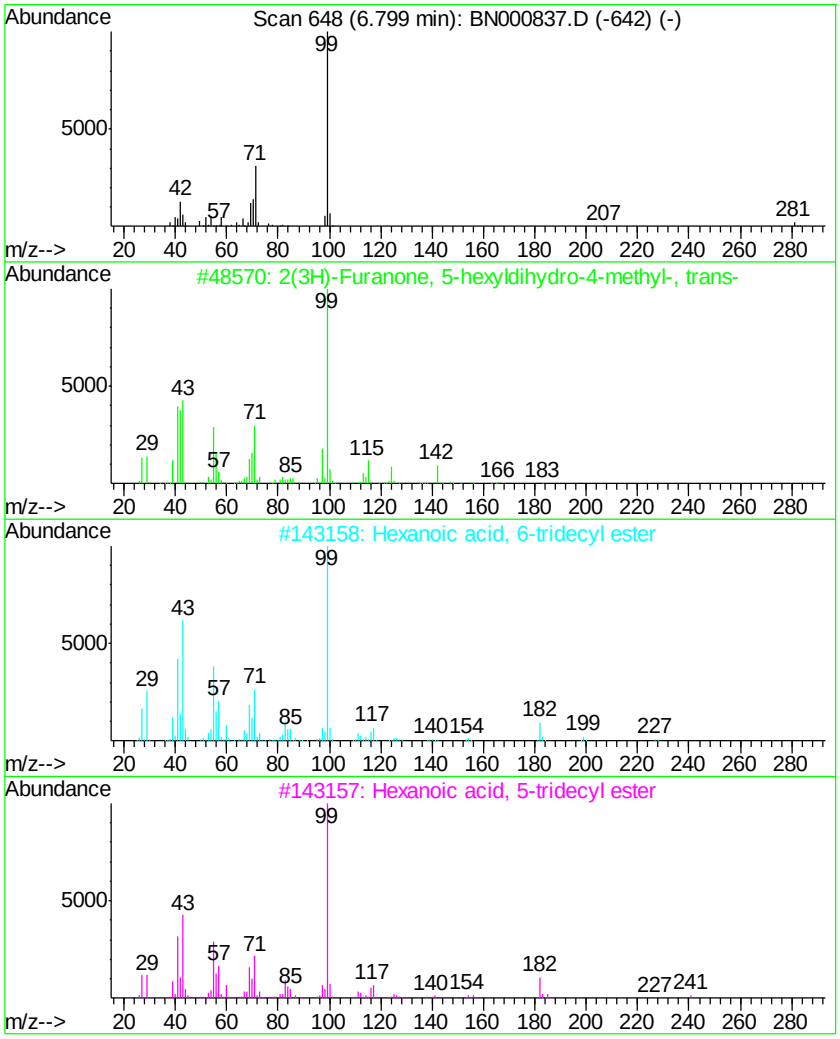
Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

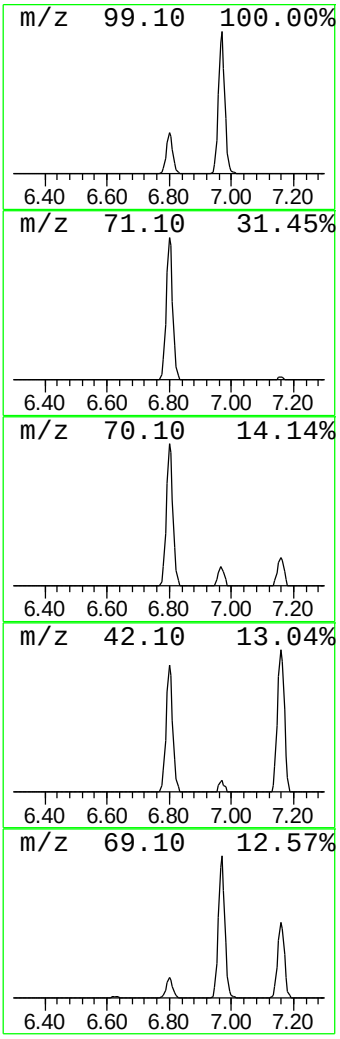
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2(3H)-Furanone, 5-hexyldihy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.80	5.95 ng/ul	281552	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, 5-hexyldihydro-4...	184	C11H20O2	147254-33-9	64
2	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	56
3	Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	56
4	Hexanoic acid, 3-tridecyl ester	298	C19H38O2	1000279-29-2	56
5	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
Data File : BN000837.D
Acq On : 23 Apr 2018 21:01
Operator : JU/SJ
Sample : J2467-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : A3XZ9

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

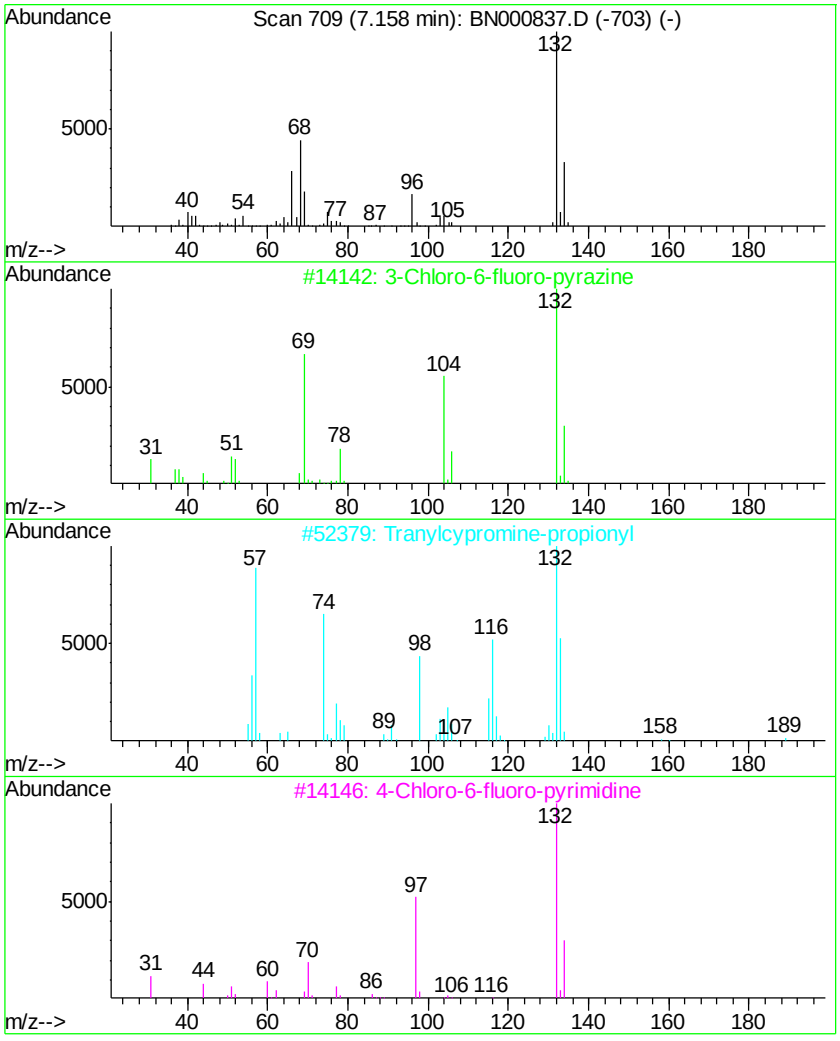
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

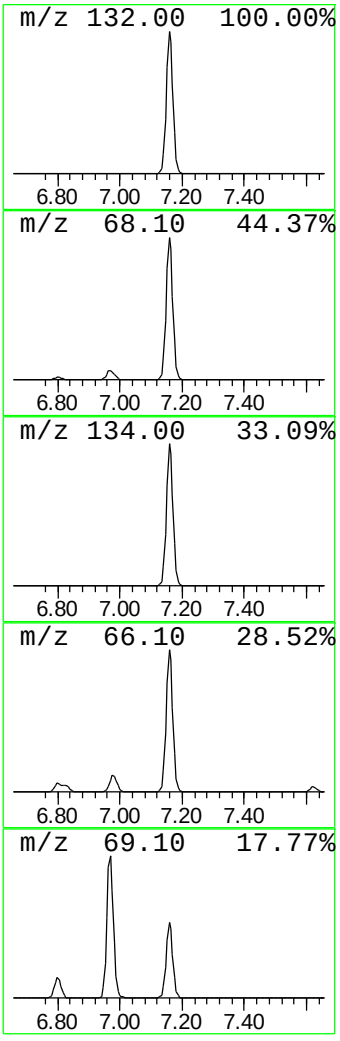
****

Peak Number 3 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	20.25 ng/ul	958467	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
Data File : BN000837.D
Acq On : 23 Apr 2018 21:01
Operator : JU/SJ
Sample : J2467-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : A3XZ9

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

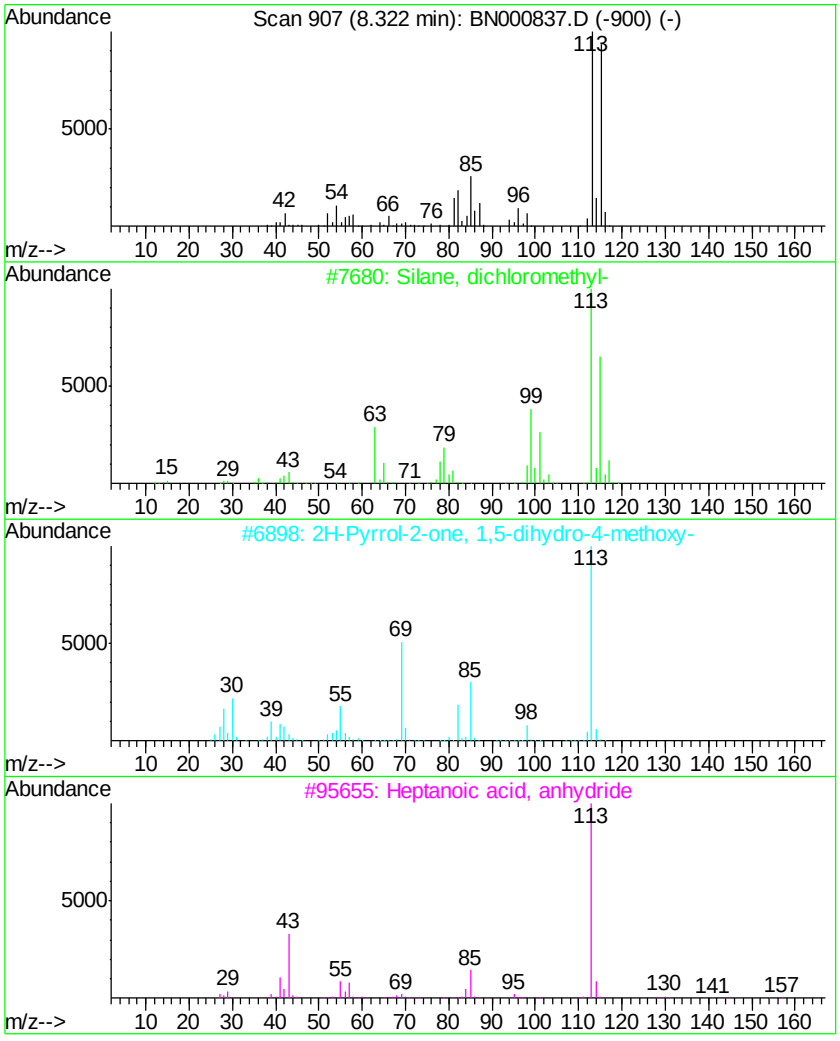
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

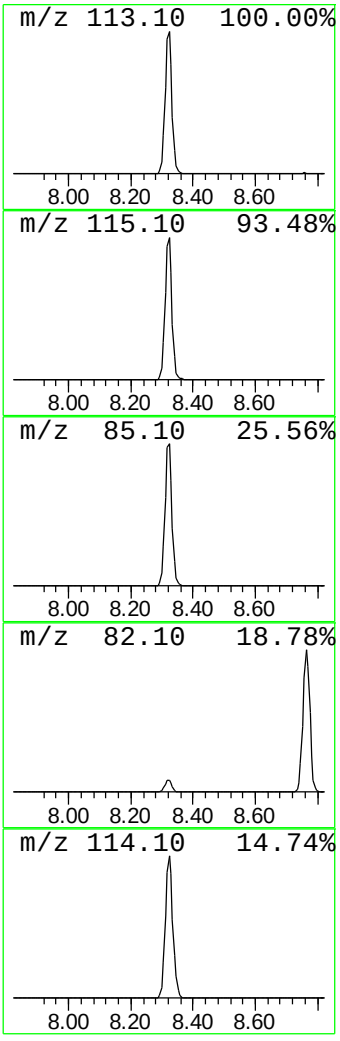
****

Peak Number 4 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.32	16.39 ng/ul	775756	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, dichloromethyl-	114	CH4Cl2Si	000075-54-7	38
2	2H-Pyrrol-2-one, 1,5-dihydro-4-m...	113	C5H7NO2	069778-83-2	32
3	Heptanoic acid, anhydride	242	C14H26O3	000626-27-7	27
4	2,2-Dimethylcyclopropanecarboxamide	113	C6H11NO	075885-58-4	27
5	Furazan-3-amine, 4-methoxy-	115	C3H5N3O2	078350-48-8	25





Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
Data File : BN000837.D
Acq On : 23 Apr 2018 21:01
Operator : JU/SJ
Sample : J2467-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : A3XZ9

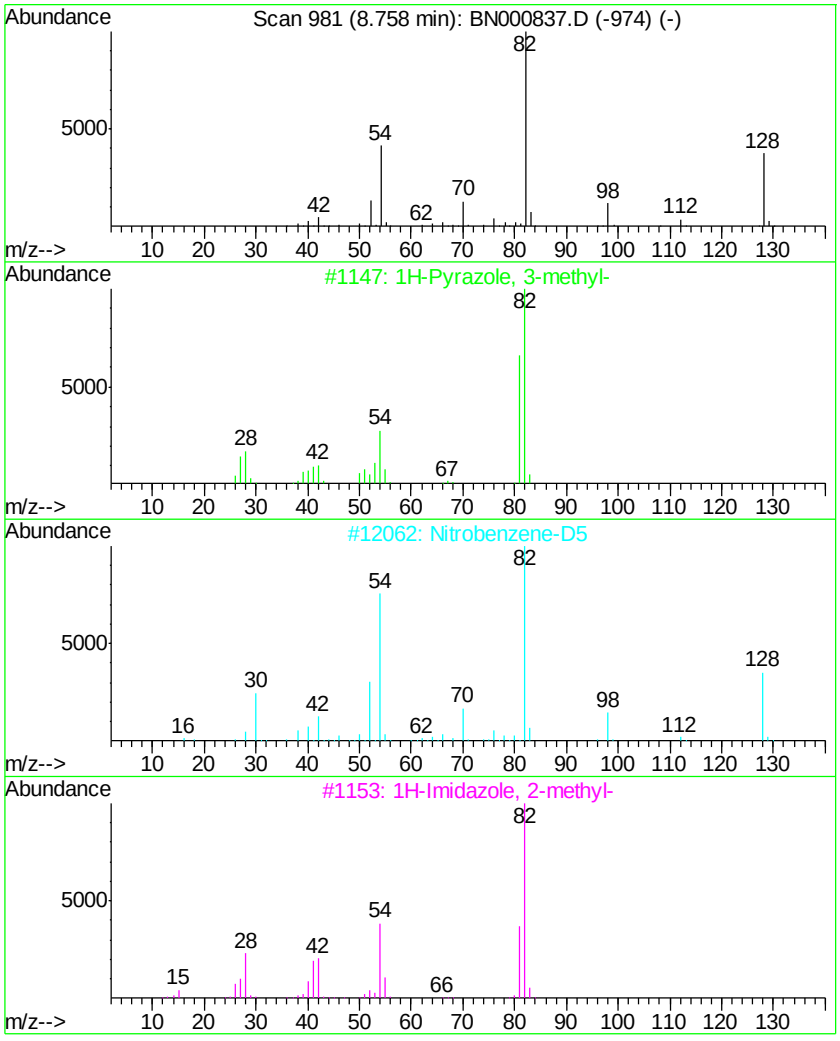
Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

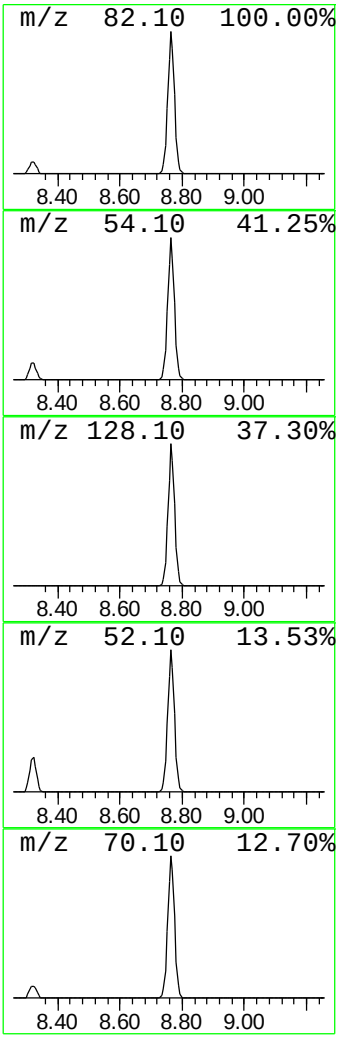
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1H-Pyrazole, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	23.50 ng/ul	1112640	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	50
2	Nitrobenzene-D5	128	C6D5NO2	004165-60-0	38
3	1H-Imidazole, 2-methyl-	82	C4H6N2	000693-98-1	38
4	Nitrobenzene-D5	128	C6D5NO2	004165-60-0	37
5	1H-Imidazole, 2-methyl-	82	C4H6N2	000693-98-1	33





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Sample : J2467-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : A3XZ9

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

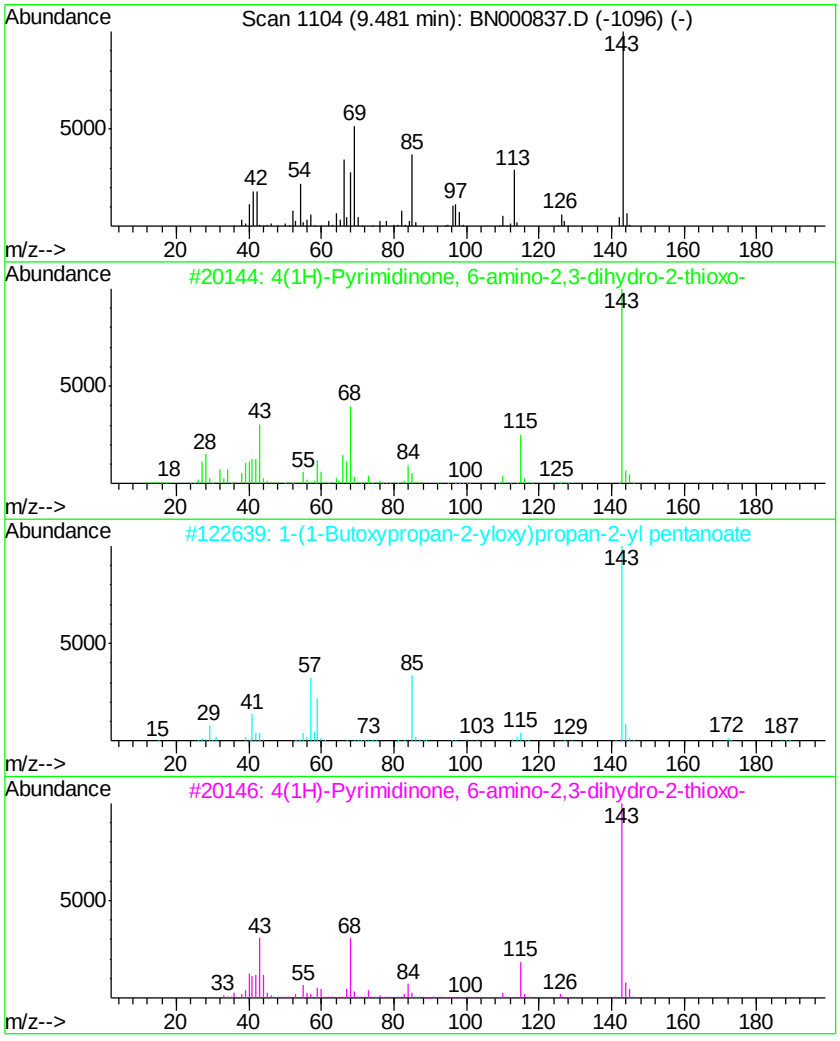
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

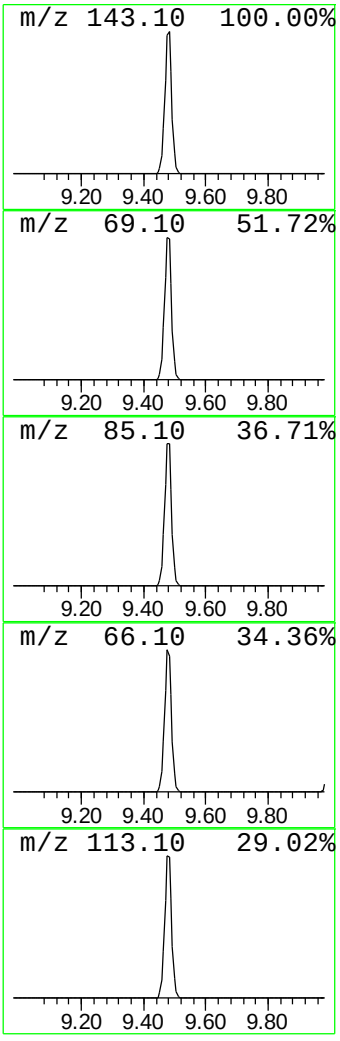
****

Peak Number 6 unknown-03 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.48	12.83 ng/ul	903213	Naphthalene-d8	10.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4(1H)-Pyrimidinone, 6-amino-2,3-...	143	C4H5N3OS	001004-40-6	12
2	1-(1-Butoxypropan-2-yloxy)propan...	274	C15H30O4	1000367-13-0	12
3	4(1H)-Pyrimidinone, 6-amino-2,3-...	143	C4H5N3OS	001004-40-6	12
4	1-(1-Butoxypropan-2-yloxy)propan...	274	C15H30O4	1000367-10-9	10
5	Tetramethylbutanedinitrile	136	C8H12N2	003333-52-6	10





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Instrument : BNA_N
ClientSampleId : A3XZ9

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

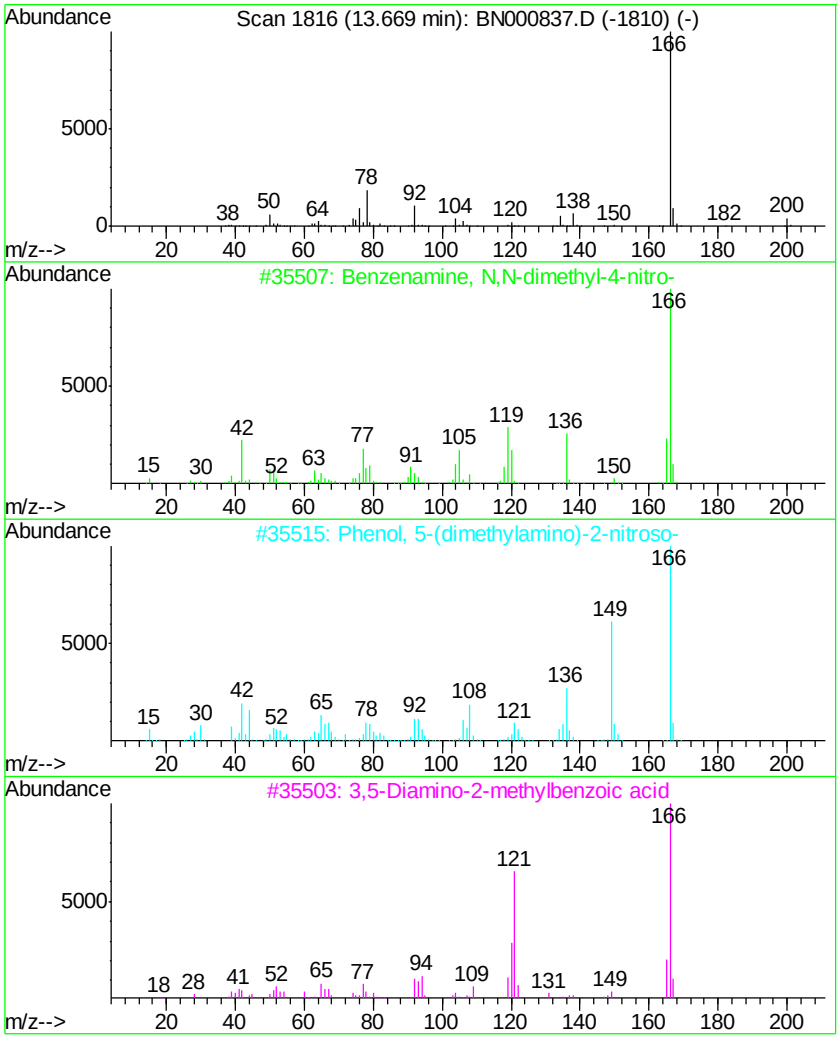
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

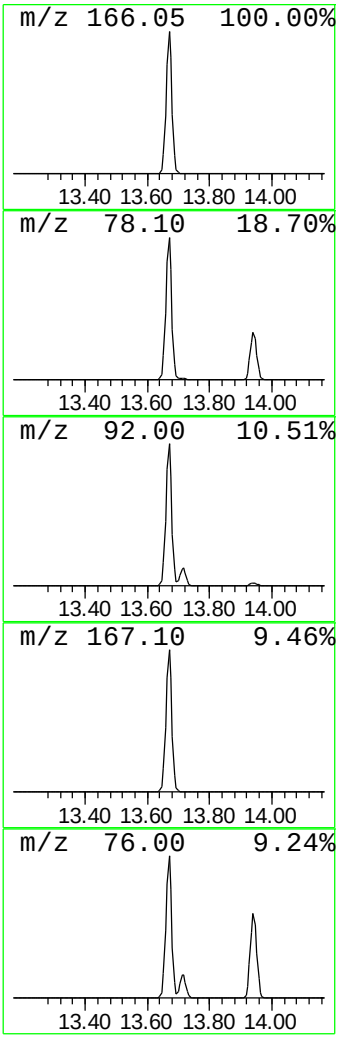
****

Peak Number 7 unknown-04 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	22.58 ng/ul	1982540	Acenaphthene-d10	14.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, N,N-dimethyl-4-nitro-	166	C8H10N2O2	000100-23-2	38
2	Phenol, 5-(dimethylamino)-2-nitr...	166	C8H10N2O2	016761-04-9	36
3	3,5-Diamino-2-methylbenzoic acid	166	C8H10N2O2	090007-30-0	36
4	6H-Purine-6-thione, 1,7-dihydro-...	166	C6H6N4S	001126-23-4	9
5	Benzo[b]tetrahydrofuran-3-one, 5...	166	C8H6O4	014771-00-7	9





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Sample : J2467-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : A3XZ9

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

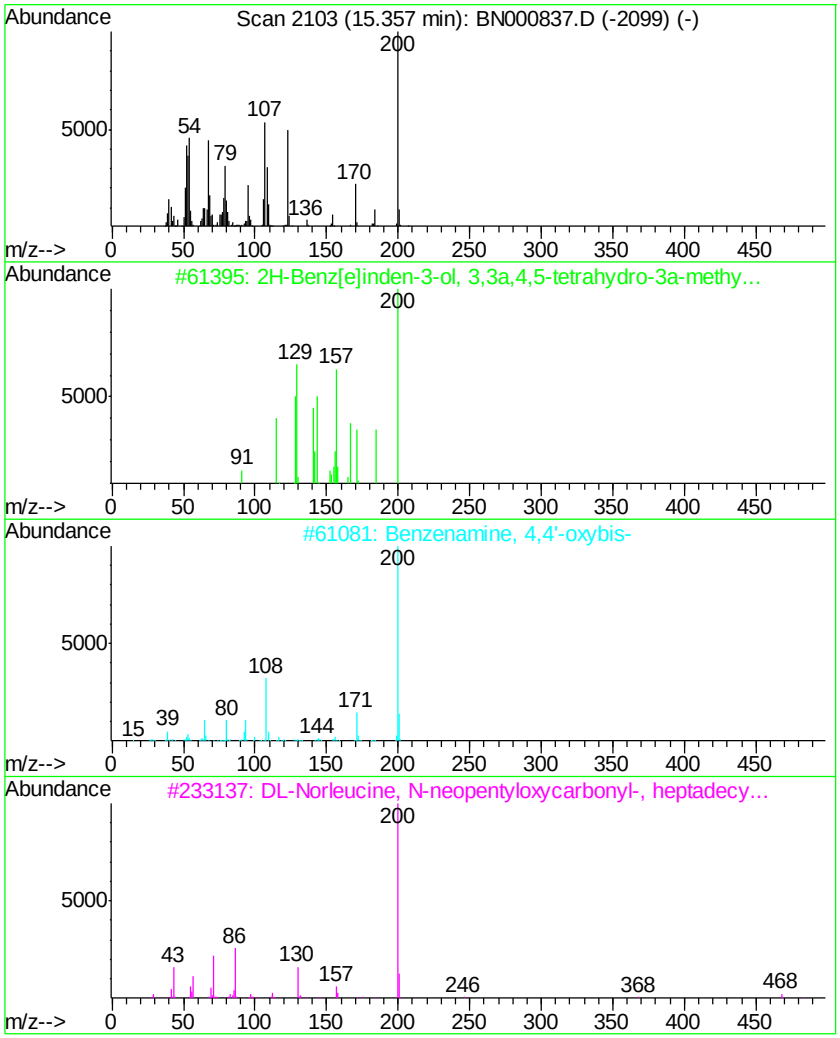
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

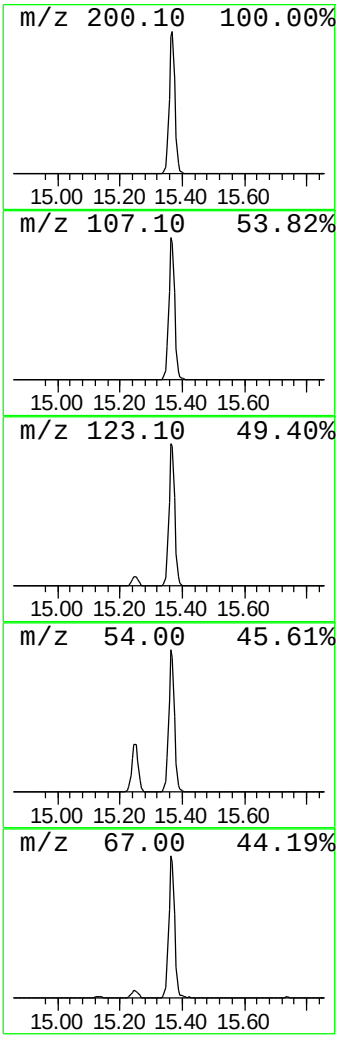
****

Peak Number 9 unknown-05 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	9.71 ng/ul	852887	Acenaphthene-d10	14.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Benz[e]inden-3-ol, 3,3a,4,5-t...	200	C14H16O	071805-91-9	22
2	Benzenamine, 4,4'-oxybis-	200	C12H12N2O	000101-80-4	11
3	DL-Norleucine, N-neopentyloxycar...	483	C29H57NO4	1000339-05-9	10
4	Benzenamine, 4,4'-oxybis-	200	C12H12N2O	000101-80-4	10
5	l-Isoleucine, N-neopentyloxycarb...	483	C29H57NO4	1000328-13-3	10





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA 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(3H)-Furanone, 5...	6.80	6.0	ng/ul	281552	1	7.62	946753	20.0
unknown-01	7.16	20.3	ng/ul	958467	1	7.62	946753	20.0
unknown-02	8.32	16.4	ng/ul	775756	1	7.62	946753	20.0
1H-Pyrazole, 3-me...	8.76	23.5	ng/ul	1112640	1	7.62	946753	20.0
unknown-03	9.48	12.8	ng/ul	903213	2	10.39	1408420	20.0
unknown-04	13.67	22.6	ng/ul	1982540	3	14.25	1755940	20.0
unknown-05	15.36	9.7	ng/ul	852887	3	14.25	1755940	20.0