LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015888.D
Acq On : 11 Jul 2018 14:39
Operator : SJ/JU
Sample : J3925-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

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_M\METHODS\8270-BM070518.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	5.316	337	345	355	rBV	89766	149737	3.03%	0.513%
2	5.798	421	427	440	rBV	784133	1248616	25.31%	4.276%
3	7.445	701	707	723	rBV	461872	840527	17.04%	2.878%
4	7.816	763	770	782	rBV	1636299	2654542	53.80%	9.090%
5	8.292	845	851	857	rBV	375895	604918	12.26%	2.071%
6	8.616	899	906	923	rVB	1591273	2530475	51.29%	8.665%
7	9.480	1046	1053	1067	rBV	1239805	2030138	41.14%	6.952%
8	11.122	1324	1332	1340	rBV	454952	770652	15.62%	2.639%
9	12.063	1486	1492	1504	rBV	49064	99739	2.02%	0.342%
10	13.539	1736	1743	1751	rBV	2891447	4055516	82.19%	13.888%
11	13.751	1773	1779	1793	rVB	400126	590991	11.98%	2.024%
12	14.363	1876	1883	1889	rBV	227350	321584	6.52%	1.101%
13	14.915	1967	1977	1987	rBV2	578980	906508	18.37%	3.104%
14	15.521	2076	2080	2085	rBV	60819	75244	1.52%	0.258%
15	16.392	2221	2228	2239	rBV	2250896	3113864	63.11%	10.663%
16	17.639	2435	2440	2449	rBV	690938	1022553	20.72%	3.502%
17	18.368	2559	2564	2570	rBV2	36266	55908	1.13%	0.191%
18	18.480	2576	2583	2588	rBV	233836	343881	6.97%	1.178%
19	18.562	2593	2597	2602	rVB	36273	53175	1.08%	0.182%
20	19.068	2678	2683	2692	rBV2	34921	49402	1.00%	0.169%
21	19.309	2720	2724	2731	rBV	55889	74038	1.50%	0.254%
22	19.615	2768	2776	2782	rBV9	34953	103162	2.09%	0.353%
23	19.727	2790	2795	2802	rBV	135479	193837	3.93%	0.664%
24	20.203	2870	2876	2884	rVB	4124785	4934117	100.00%	16.896%
25	21.503	3093	3097	3105	rBV	272714	354773	7.19%	1.215%
26	21.750	3134	3139	3145	rBV	799584	1053102	21.34%	3.606%
27	24.144	3540	3546	3556	rVB	482220	971076	19.68%	3.325%

Sum of corrected areas: 29202075

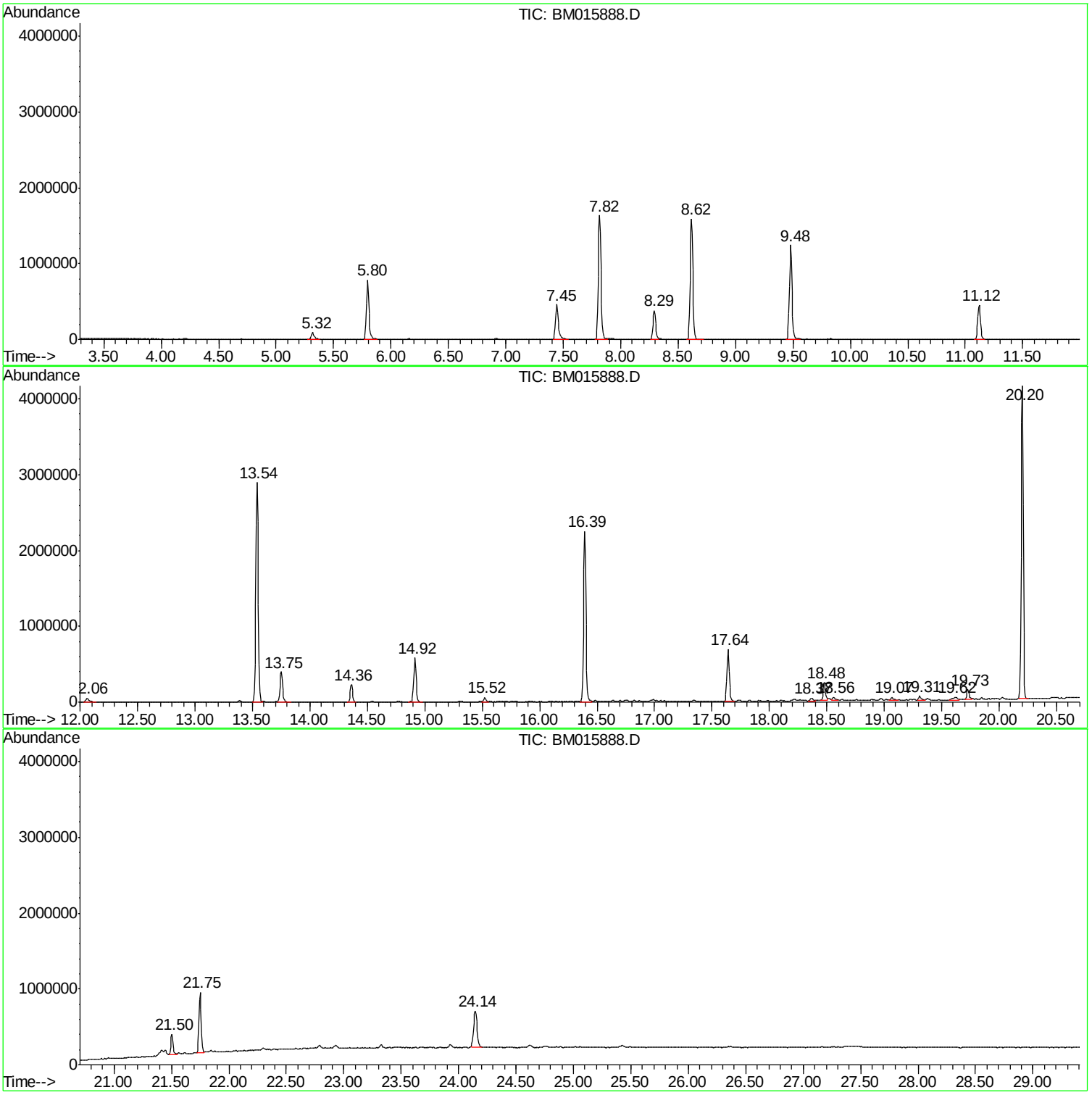
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015888.D
Acq On : 11 Jul 2018 14:39
Operator : SJ/JU
Sample : J3925-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015888.D
Acq On : 11 Jul 2018 14:39
Operator : SJ/JU
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

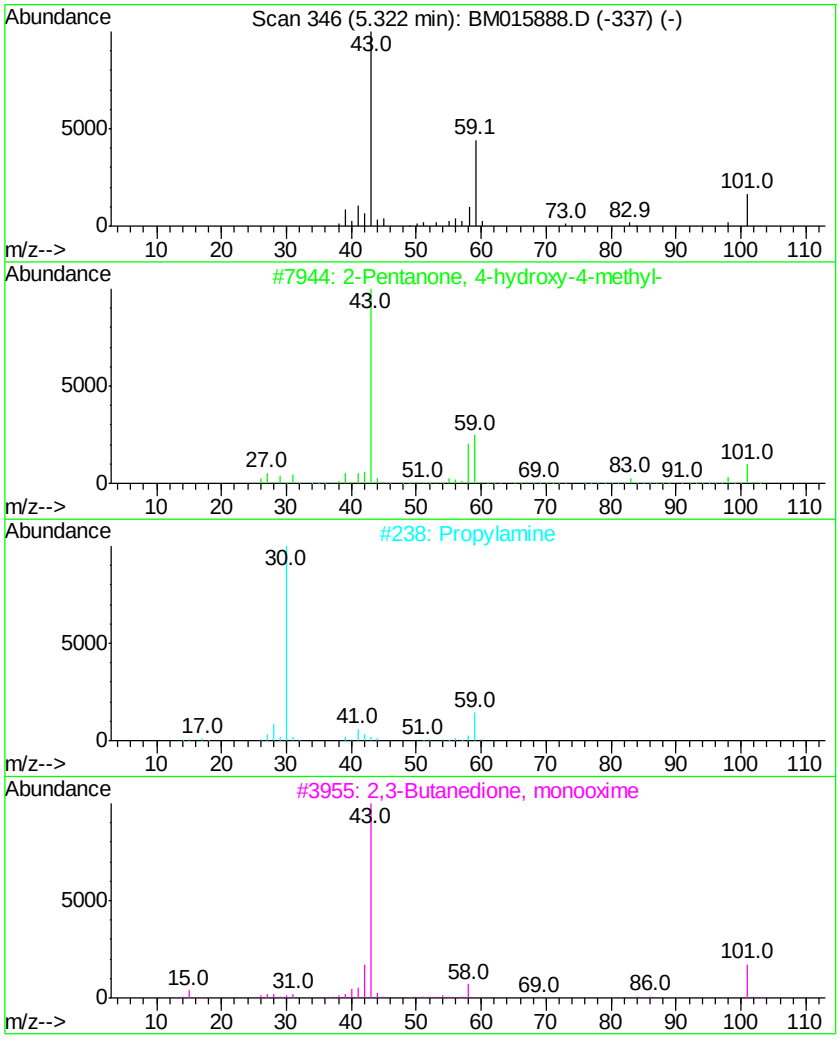
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

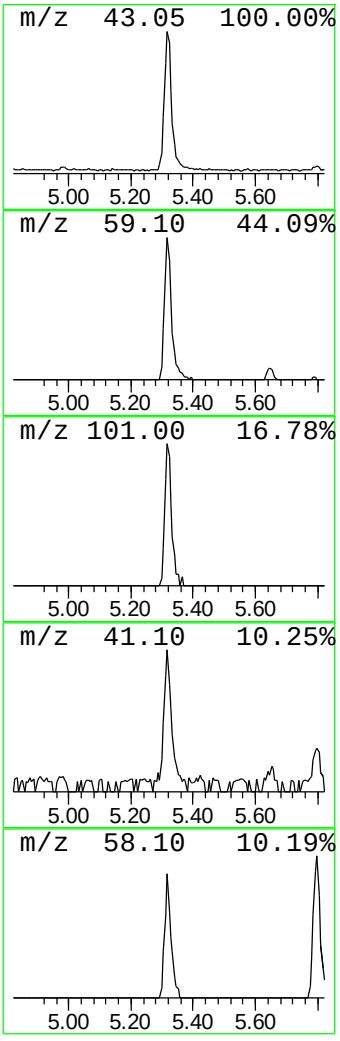
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	4.95 ng	149737	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propylamine	59	C3H9N	000107-10-8	40
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9





Library Search Compound Report

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Data File : BM015888.D
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Operator : SJ/JU
Sample : J3925-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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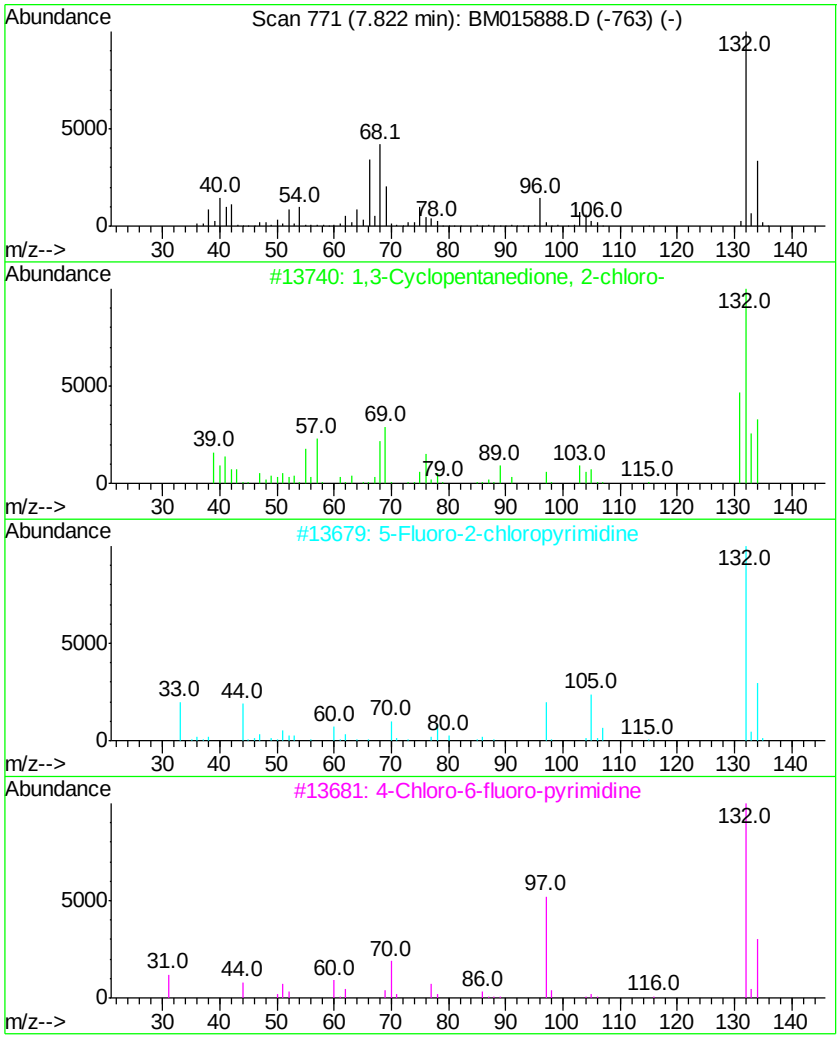
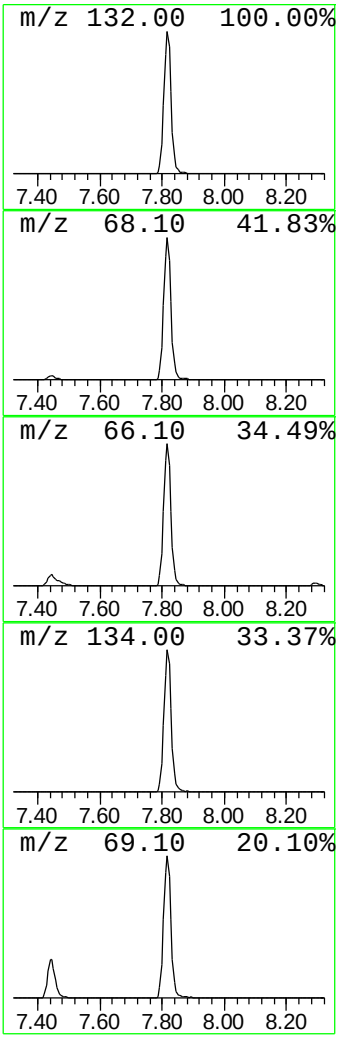
Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	87.77 ng	2654540	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015888.D
Acq On : 11 Jul 2018 14:39
Operator : SJ/JU
Sample : J3925-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

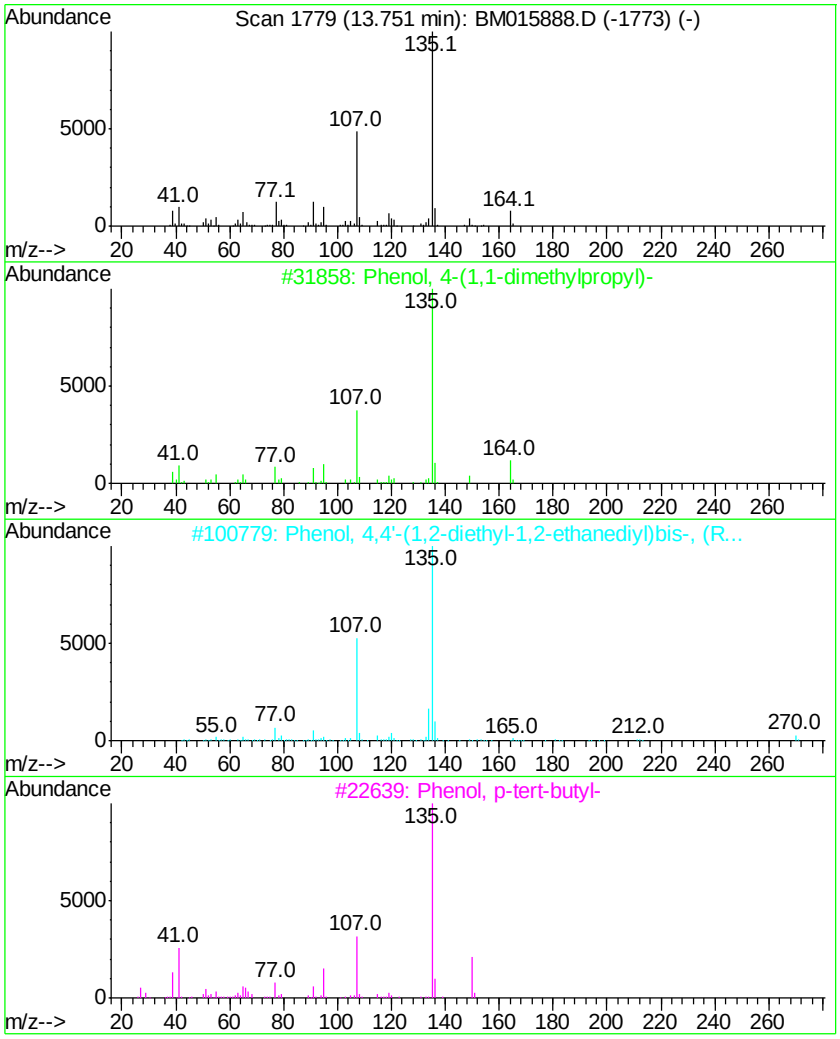
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

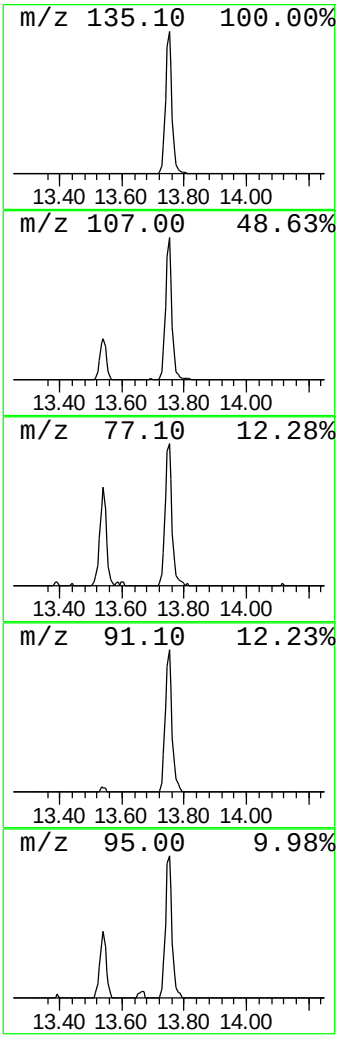
****

Peak Number 4 Phenol, 4-(1,1-dimethylprop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	13.04 ng	590991	Acenaphthene-d10	14.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, 4,4'-(1,2-diethyl-1,2-et...	270	C18H22O2	000084-16-2	72
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64
4	2-Aziridinone, 1-(1-adamantyl)-3...	273	C18H27NO	026905-18-0	53
5	Hexestrol	270	C18H22O2	005635-50-7	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015888.D
Acq On : 11 Jul 2018 14:39
Operator : SJ/JU
Sample : J3925-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

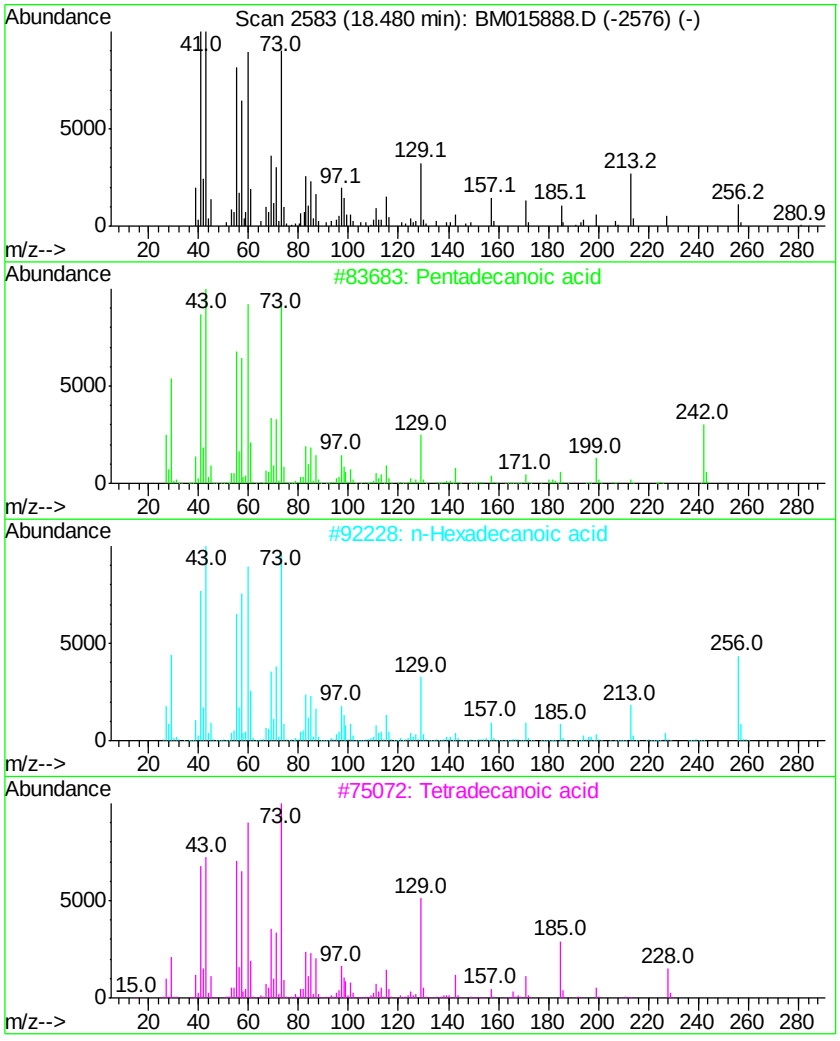
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

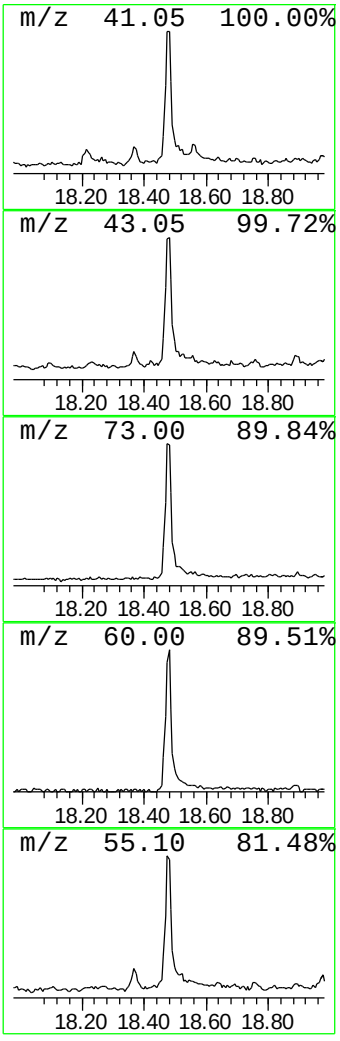
****

Peak Number 5 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.48	6.73 ng	343881	Phenanthrene-d10	17.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
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Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

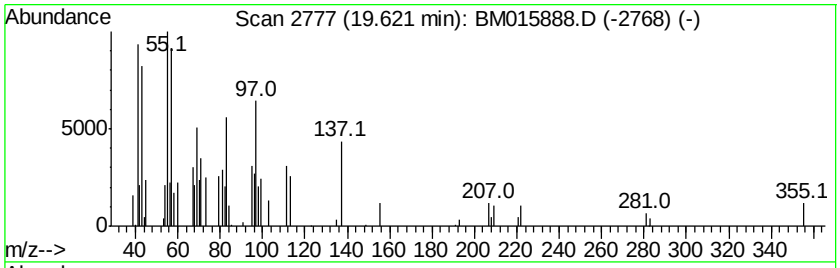
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

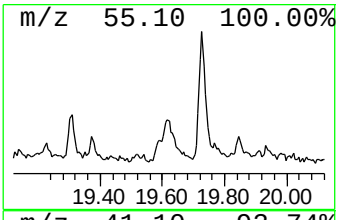
****

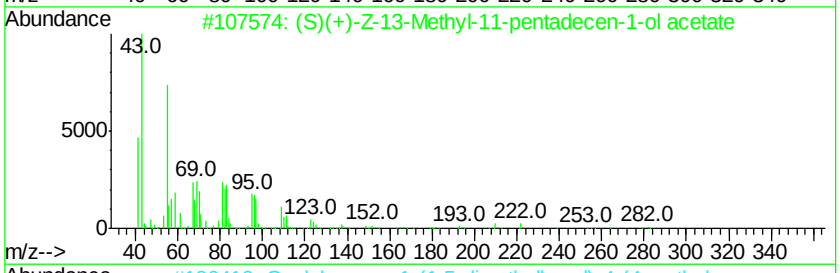
Peak Number 6 (S)(+)-Z-13-Methyl-11-penta... Concentration Rank 8

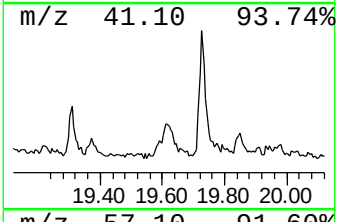
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	2.02 ng	103162	Phenanthrene-d10	17.64

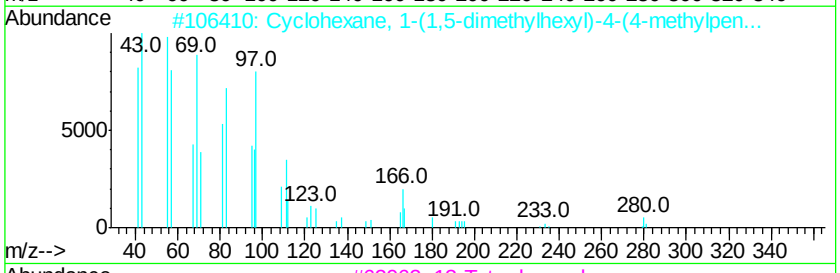
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)(+)-Z-13-Methyl-11-pentadecen...	282	C18H34O2	1000130-84-8	60
2	Cyclohexane, 1-(1,5-dimethylhexy...	280	C20H40	056009-20-2	47
3	13-Tetradecenal	210	C14H26O	085896-31-7	46
4	13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	46
5	2-Bromopropionic acid, 1-(cyclop...	248	C10H17BrO2	1000293-39-1	43

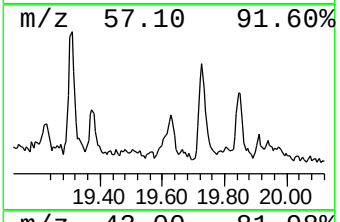


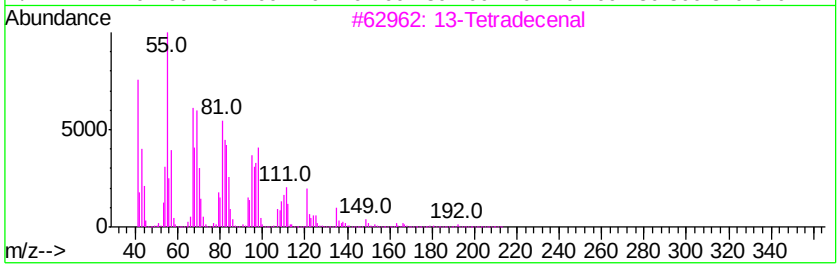


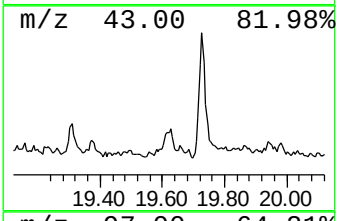


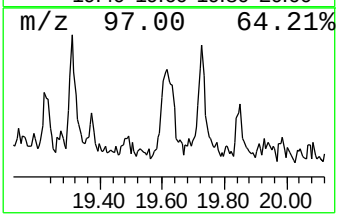












Library Search Compound Report

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Sample : J3925-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

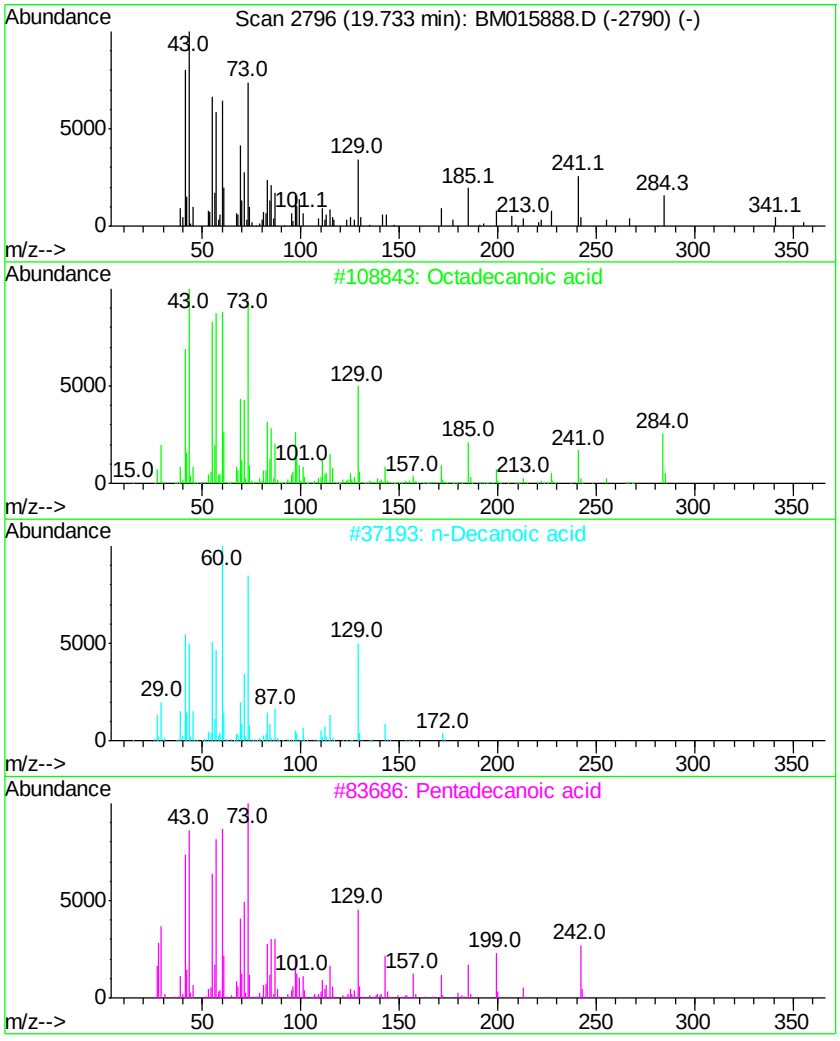
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

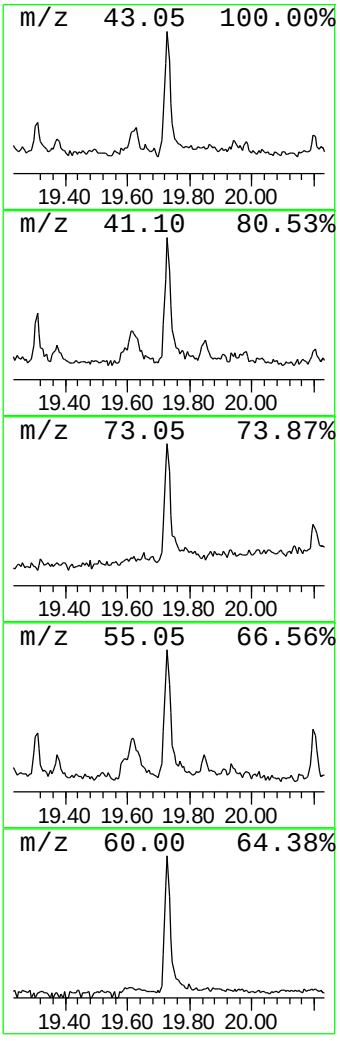
****

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	3.68 ng	193837	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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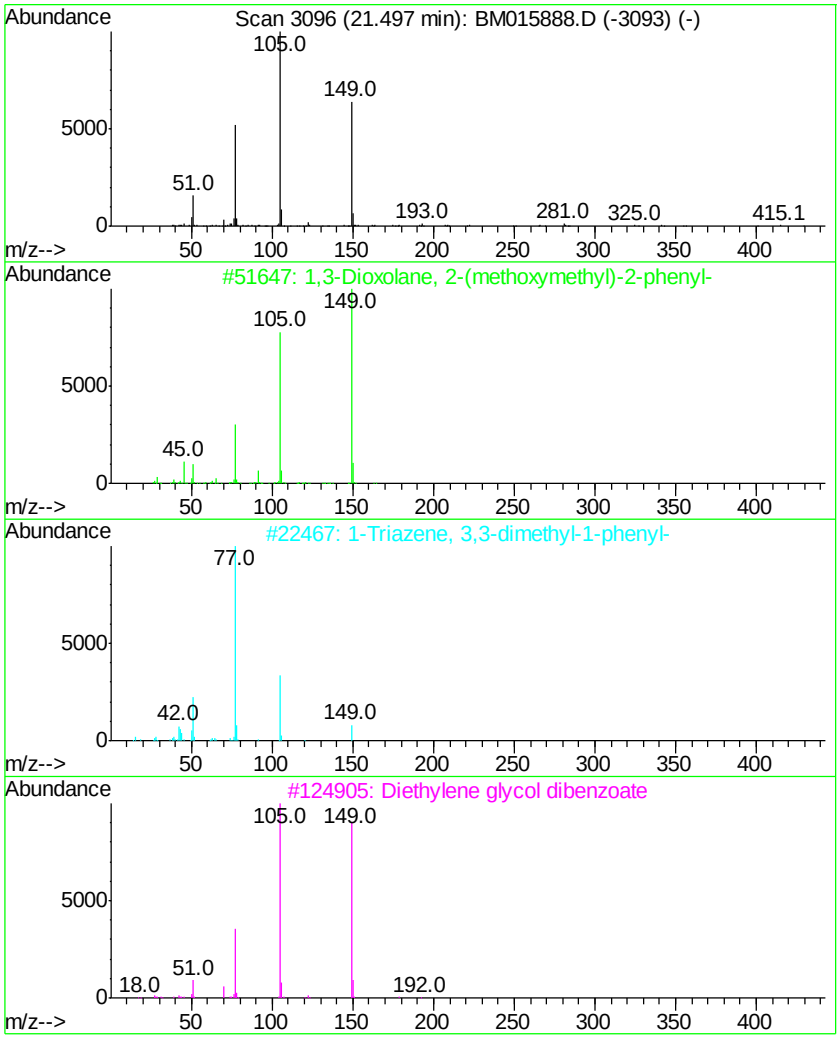
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

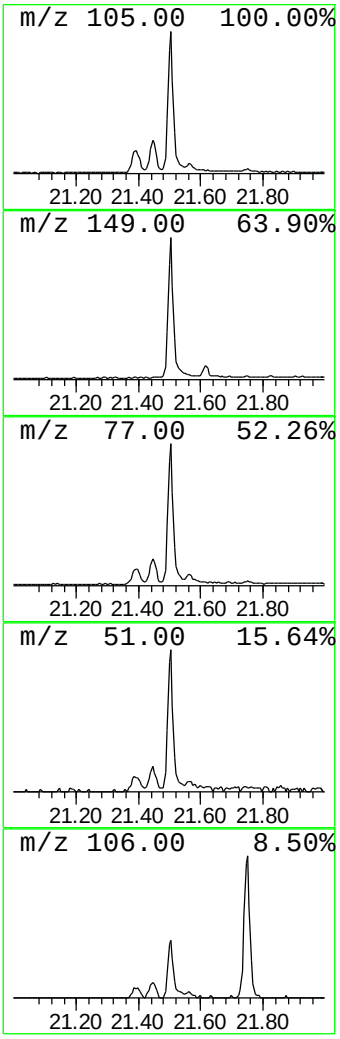
****

Peak Number 8 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	6.74 ng	354773	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	78
2	1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	72
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
4	Ethanone, 2-chloro-1,2-diphenyl-	230	C14H11ClO	000447-31-4	43
5	Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM071118\
Data File : BM015888.D
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Misc :
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Instrument : BNA_M
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.32	5.0	ng	149737	1	8.29	604918	20.0
unknown7.82	7.82	87.8	ng	2654540	1	8.29	604918	20.0
Phenol, 4-(1,1-di...	13.75	13.0	ng	590991	3	14.92	906508	20.0
Pentadecanoic acid	18.48	6.7	ng	343881	4	17.64	1022550	20.0
(S)(+)-Z-13-Methy...	19.62	2.0	ng	103162	4	17.64	1022550	20.0
Octadecanoic acid	19.73	3.7	ng	193837	5	21.75	1053100	20.0
1,3-Dioxolane, 2-...	21.50	6.7	ng	354773	5	21.75	1053100	20.0