LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
Data File : BM016256.D
Acq On : 08 Aug 2018 18:55
Operator : SJ/JU
Sample : J4313-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-13

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-BM072318.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	5.187	318	323	330	rBV	130003	188571	12.04%	1.201%
2	5.663	398	404	415	rBV	709867	1066875	68.09%	6.797%
3	7.304	676	683	698	rBV	672999	1095482	69.92%	6.979%
4	7.663	738	744	757	rBV	770010	1222328	78.02%	7.787%
5	8.134	818	824	835	rBV	201956	330822	21.11%	2.108%
6	8.457	872	879	890	rBV	584911	938444	59.90%	5.979%
7	9.322	1019	1026	1044	rBV	407959	692952	44.23%	4.415%
8	10.951	1297	1303	1311	rBV	233398	379706	24.23%	2.419%
9	13.392	1712	1718	1728	rBV	873033	1236673	78.93%	7.879%
10	14.227	1855	1860	1866	rBB	47172	66062	4.22%	0.421%
11	14.774	1947	1953	1959	rBV2	258324	393547	25.12%	2.507%
12	14.833	1959	1963	1970	rVB	13960	18198	1.16%	0.116%
13	15.816	2124	2130	2136	rBV	13062	15752	1.01%	0.100%
14	16.257	2200	2205	2217	rBV	648571	901033	57.51%	5.740%
15	16.474	2238	2242	2249	rVB	23629	33528	2.14%	0.214%
16	17.504	2412	2417	2421	rBV	291314	416233	26.57%	2.652%
17	17.551	2421	2425	2430	rVB	206325	287182	18.33%	1.830%
18	17.639	2436	2440	2446	rVB	41373	56877	3.63%	0.362%
19	17.921	2481	2488	2492	rBV2	17524	28825	1.84%	0.184%
20	18.357	2557	2562	2569	rBV3	76573	142108	9.07%	0.905%
21	18.421	2569	2573	2581	rVB2	37919	57643	3.68%	0.367%
22	18.504	2581	2587	2591	rBV2	12958	19198	1.23%	0.122%
23	18.568	2591	2598	2602	rBV2	35914	66968	4.27%	0.427%
24	18.604	2602	2604	2607	rVB	17804	16915	1.08%	0.108%
25	18.862	2642	2648	2652	rBV3	18620	24391	1.56%	0.155%
26	18.927	2655	2659	2664	rBV3	18389	27376	1.75%	0.174%
27	19.274	2709	2718	2721	rBV5	20264	32210	2.06%	0.205%
28	19.427	2741	2744	2748	rVB3	12882	18468	1.18%	0.118%
29	19.539	2758	2763	2769	rVB	380446	498340	31.81%	3.175%
30	19.615	2770	2776	2786	rBV7	33168	57500	3.67%	0.366%
31	19.868	2814	2819	2821	rBV2	62795	92726	5.92%	0.591%
32	19.904	2821	2825	2832	rVV	332170	439678	28.06%	2.801%
33	19.968	2832	2836	2841	rVB2	18425	29959	1.91%	0.191%
34	20.086	2851	2856	2861	rBV	1360015	1566779	100.00%	9.982%

LSC Area Percent Report

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Misc :
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Instrument : BNA_M
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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-BM072318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.221	2873	2879	2886	rBV6	27627	74701	4.77%	0.476%
36	20.286	2886	2890	2894	rBV5	12042	18940	1.21%	0.121%
37	20.356	2899	2902	2904	rVV4	26214	38123	2.43%	0.243%
38	20.386	2904	2907	2913	rVB	45554	67572	4.31%	0.430%
39	20.486	2920	2924	2927	rBV	32745	41097	2.62%	0.262%
40	20.545	2927	2934	2937	rVV3	37135	68466	4.37%	0.436%
41	20.680	2954	2957	2962	rBV2	27515	41698	2.66%	0.266%
42	20.727	2962	2965	2971	rVV5	23866	41008	2.62%	0.261%
43	21.133	3030	3034	3038	rBV	45631	70919	4.53%	0.452%
44	21.309	3057	3064	3070	rBV5	100481	239723	15.30%	1.527%
45	21.633	3113	3119	3123	rBV2	488039	896873	57.24%	5.714%
46	21.674	3123	3126	3131	rVB	199153	252998	16.15%	1.612%
47	23.268	3393	3397	3403	rBV	160522	379158	24.20%	2.416%
48	23.774	3479	3483	3489	rVB	123245	214574	13.70%	1.367%
49	23.874	3496	3500	3508	rVB	159597	283765	18.11%	1.808%
50	23.974	3512	3517	3523	rBV	270122	507625	32.40%	3.234%

Sum of corrected areas: 15696589

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Instrument : BNA_M
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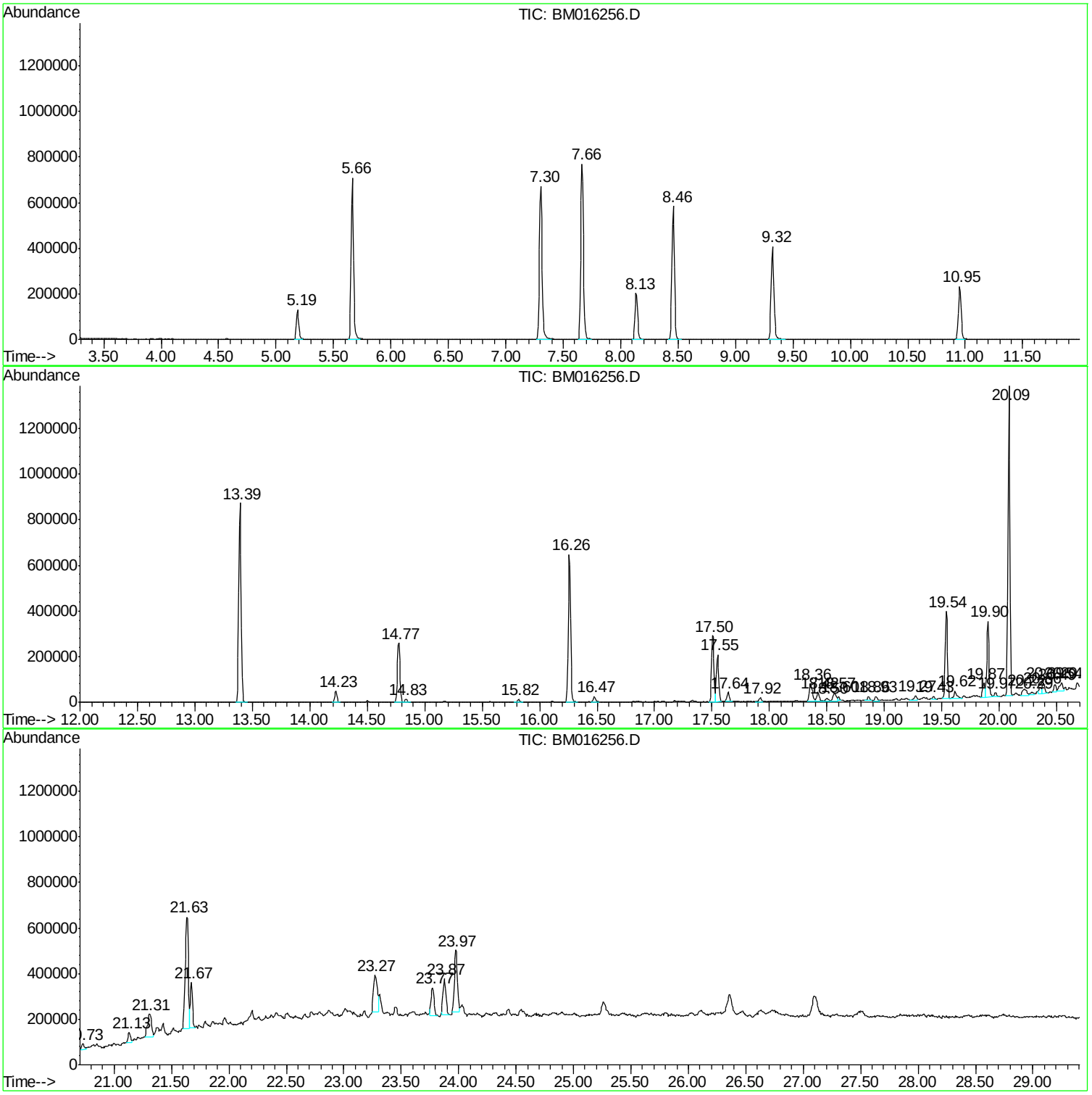
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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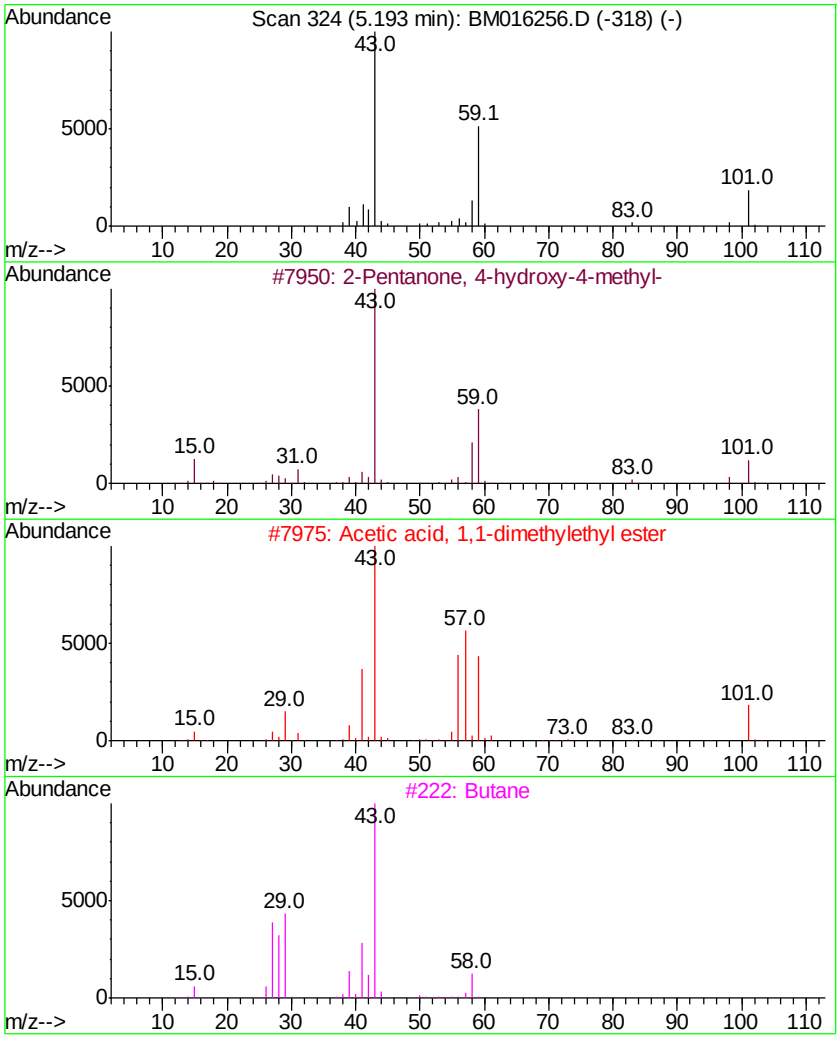
TIC Integration Parameters: LSCINT.P

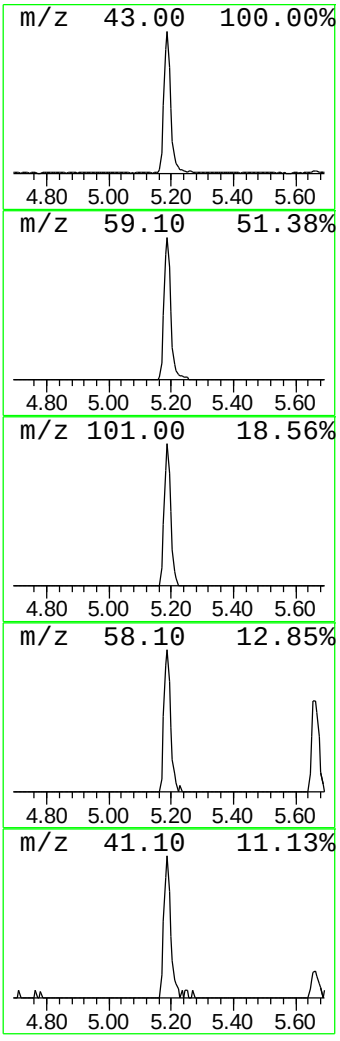
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	11.40 ng	188571	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Butane	58	C4H10	000106-97-8	22
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5	Propylamine	59	C3H9N	000107-10-8	9





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-13

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

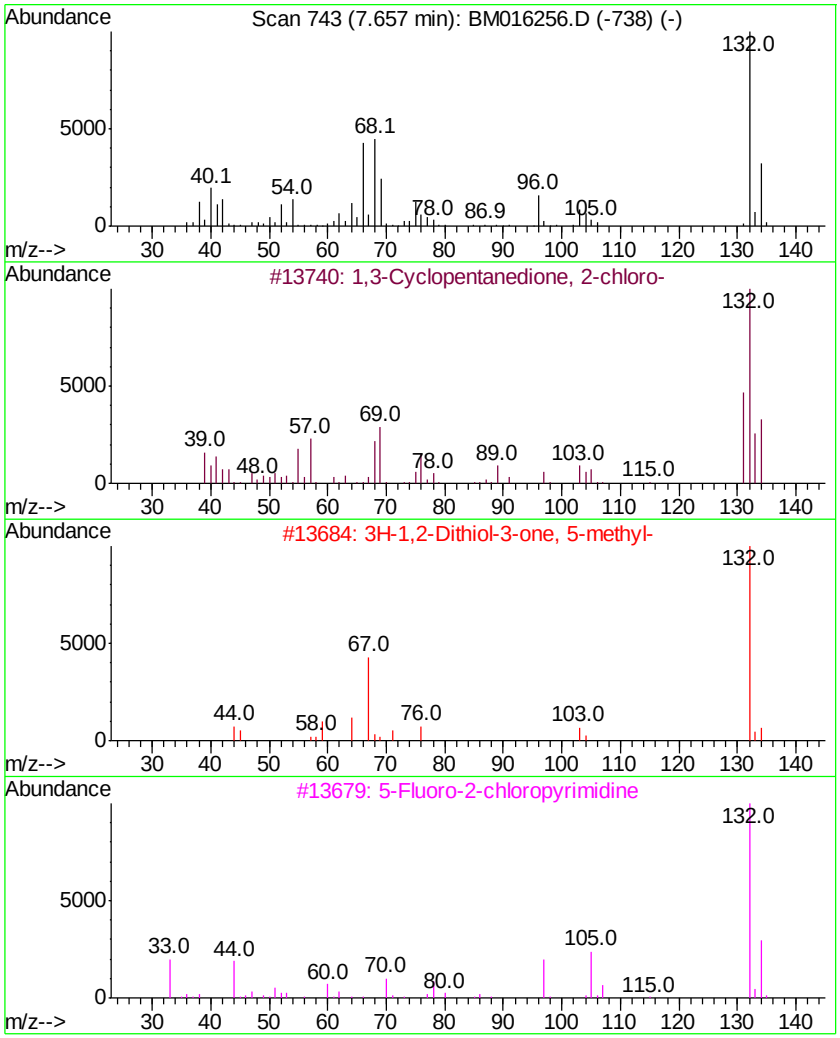
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

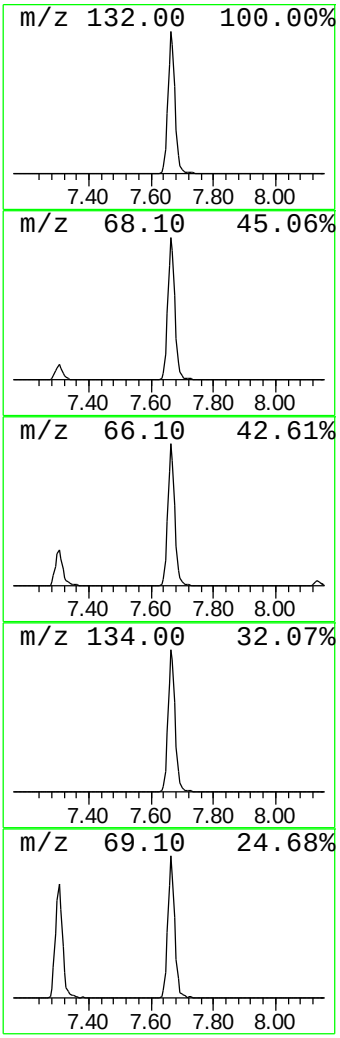
****

Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	73.90 ng	1222330	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10





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Instrument : BNA_M
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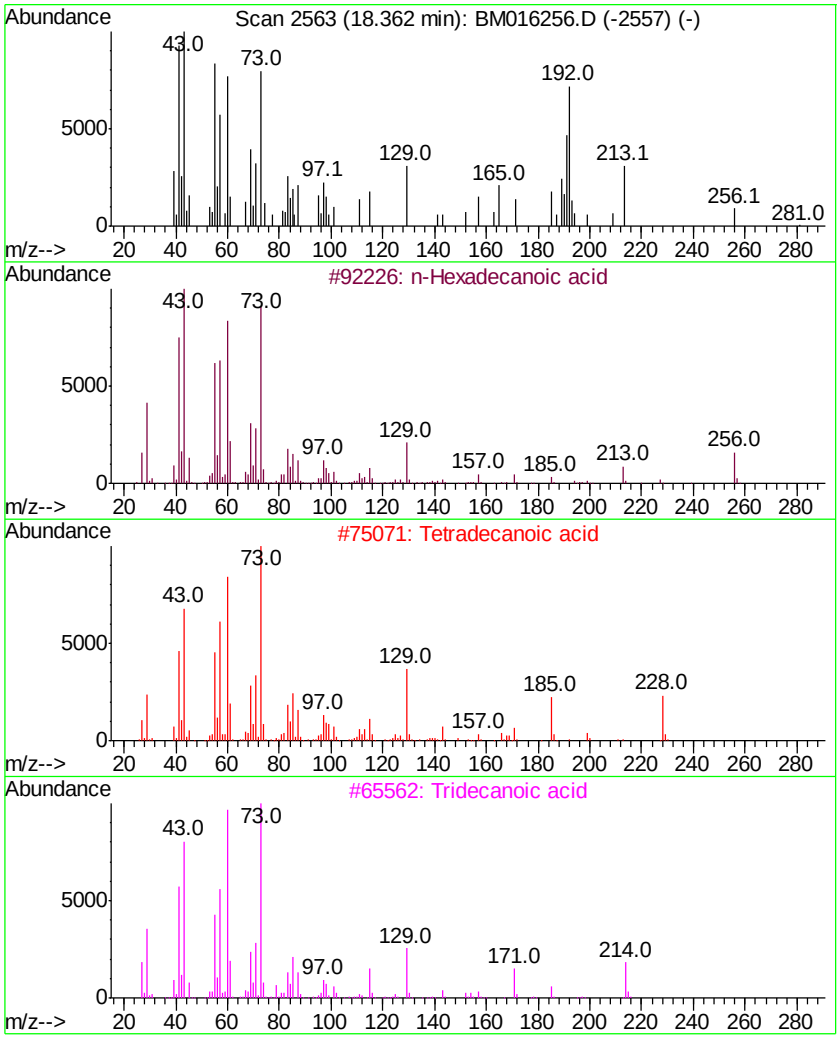
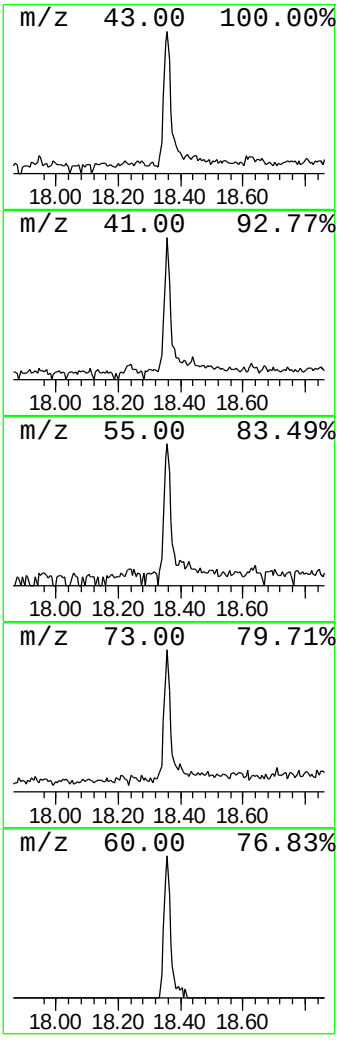
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	6.83 ng	142108	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
3	Tridecanoic acid	214	C13H26O2	000638-53-9	49
4	Undecanoic acid	186	C11H22O2	000112-37-8	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43





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Instrument : BNA_M
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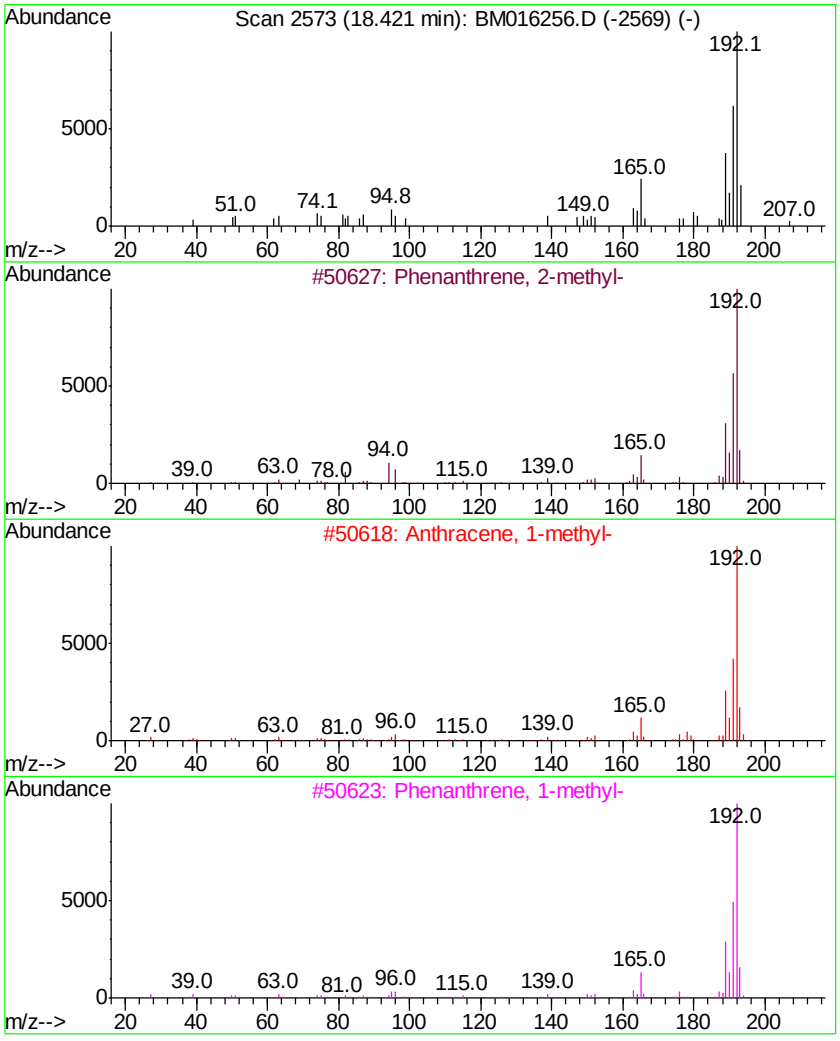
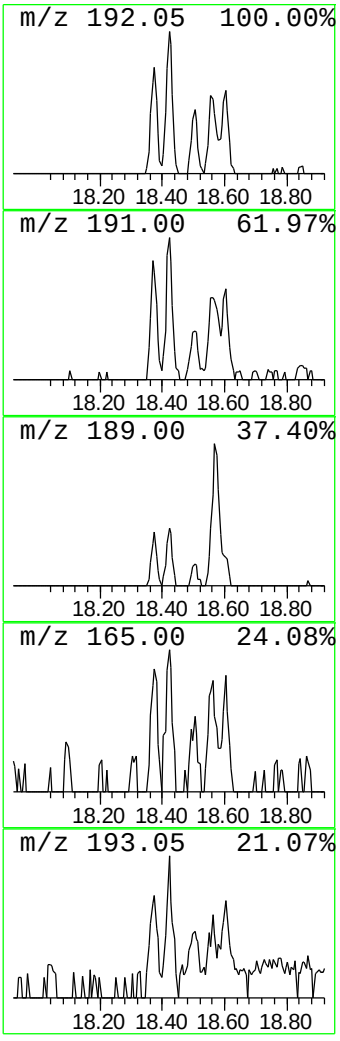
Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	2.77 ng	57643	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	89
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	87





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ClientSampleId : C-13

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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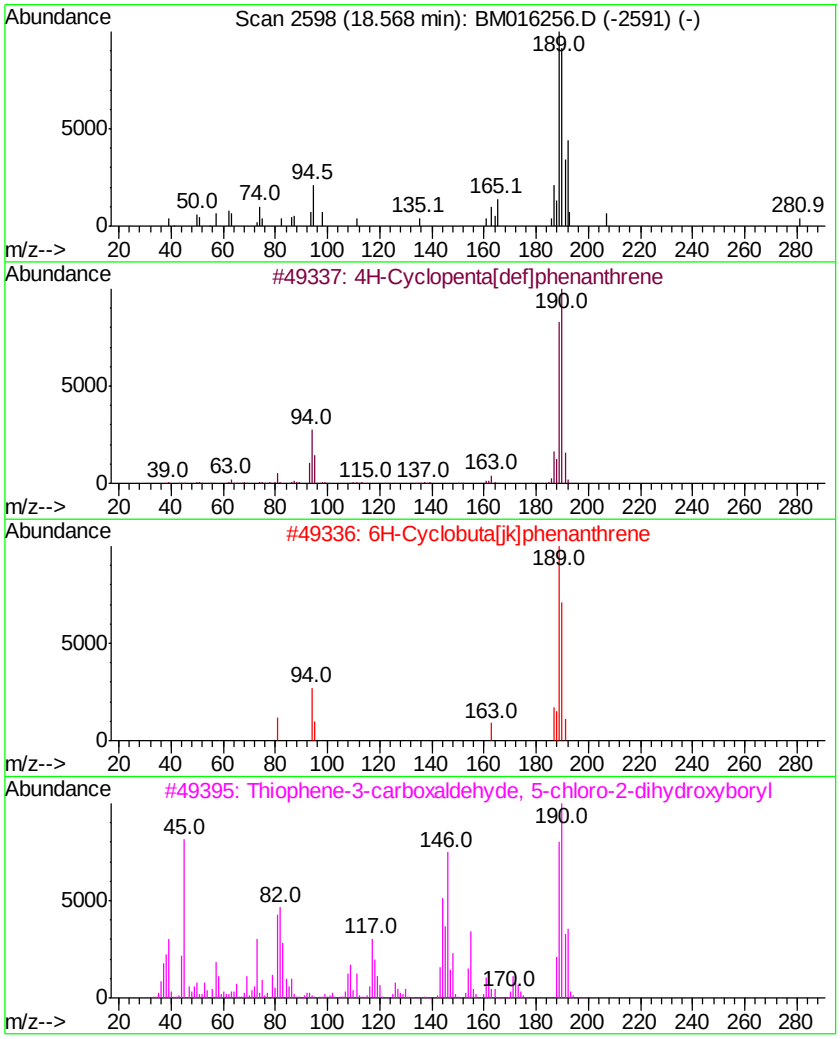
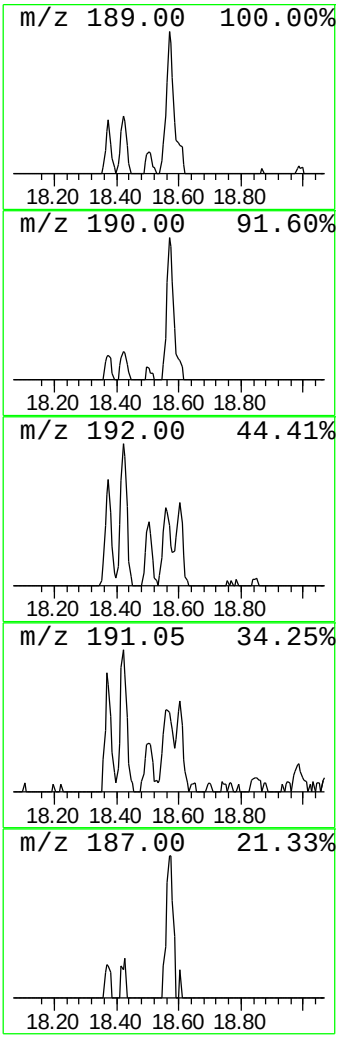
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	3.22 ng	66968	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	45
5	3H-Indazole-3-carbonitrile, 3-(4...	253	C14H8ClN3	056630-97-8	27





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Instrument : BNA_M
ClientSampleId : C-13

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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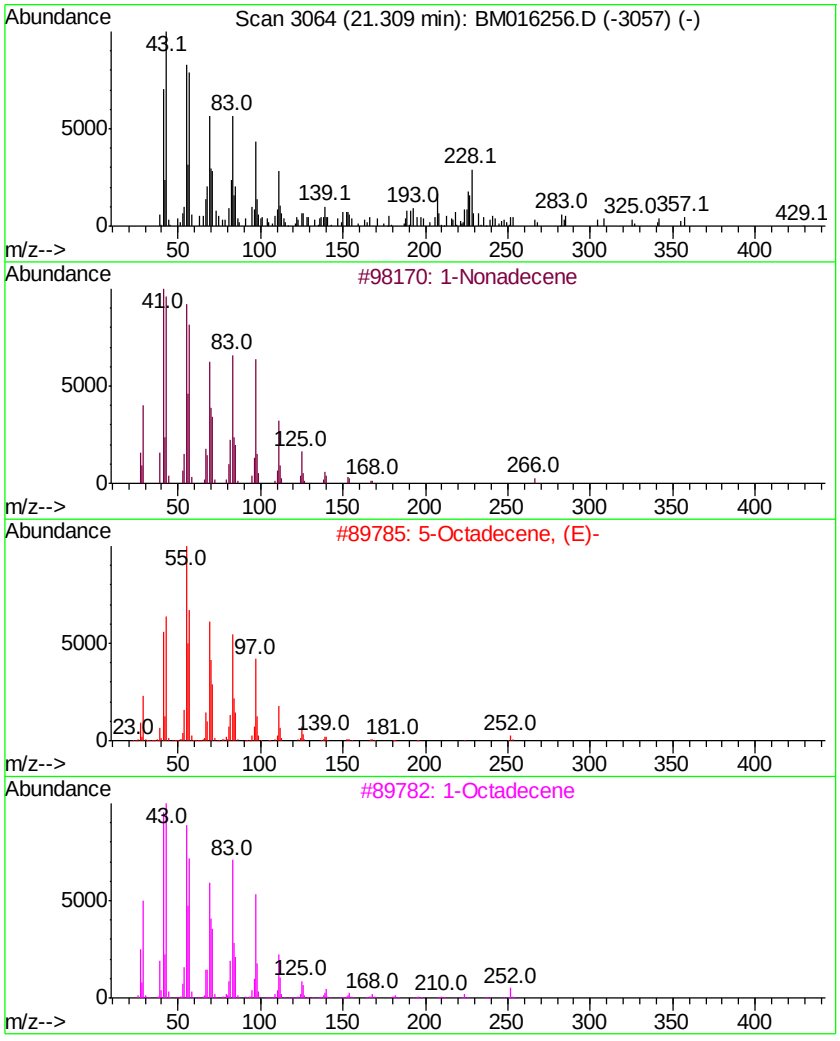
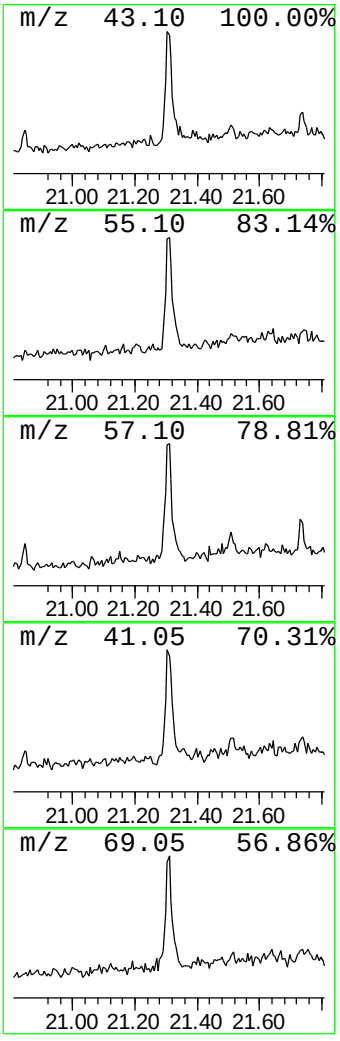
****

Peak Number 7 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	5.35 ng	239723	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	93
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	92
3	1-Octadecene	252	C18H36	000112-88-9	92
4	1-Docosene	308	C22H44	001599-67-3	92
5	1-Docosanethiol	342	C22H46S	007773-83-3	89





Tentatively Identified Compound (LSC) summary

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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...	5.19	11.4	ng	188571	1	8.14	330822	20.0
unknown7.66	7.66	73.9	ng	1222330	1	8.14	330822	20.0
n-Hexadecanoic acid	18.36	6.8	ng	142108	4	17.50	416233	20.0
Phenanthrene, 2-m...	18.42	2.8	ng	57643	4	17.50	416233	20.0
4H-Cyclopenta[def...	18.57	3.2	ng	66968	4	17.50	416233	20.0
1-Nonadecene	21.31	5.3	ng	239723	5	21.64	896873	20.0