

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
 Data File : BM016358.D
 Acq On : 14 Aug 2018 17:13
 Operator : SJ/JU
 Sample : J4427-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RB47197

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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	5.169	315	320	334	rVB	115318	173649	8.00%	1.051%
2	5.646	395	401	420	rBV	802071	1211590	55.85%	7.331%
3	7.287	674	680	701	rVB	800642	1310921	60.42%	7.932%
4	7.646	734	741	754	rBV	906555	1424978	65.68%	8.623%
5	8.116	815	821	829	rBB	172195	275195	12.68%	1.665%
6	8.434	869	875	889	rBB	621127	1010369	46.57%	6.114%
7	9.304	1016	1023	1038	rBV	492410	813928	37.52%	4.925%
8	10.928	1292	1299	1305	rBV	209291	349790	16.12%	2.117%
9	10.981	1305	1308	1314	rVB	30344	46197	2.13%	0.280%
10	13.369	1708	1714	1721	rBV	1058234	1471127	67.81%	8.902%
11	14.204	1849	1856	1862	rBV	81271	119278	5.50%	0.722%
12	14.480	1894	1903	1909	rBV	14447	28600	1.32%	0.173%
13	14.751	1943	1949	1956	rVV2	287152	431189	19.87%	2.609%
14	14.816	1956	1960	1965	rVB2	20949	32496	1.50%	0.197%
15	15.151	2011	2017	2023	rVB3	18853	30011	1.38%	0.182%
16	15.798	2121	2127	2134	rBV2	17422	31548	1.45%	0.191%
17	16.245	2196	2203	2209	rBV	1211453	1698225	78.28%	10.276%
18	16.427	2228	2234	2237	rBV5	22882	39253	1.81%	0.238%
19	16.786	2286	2295	2303	rBV9	9667	32926	1.52%	0.199%
20	17.486	2409	2414	2418	rBV	365677	532560	24.55%	3.223%
21	17.533	2418	2422	2428	rVB	144530	211458	9.75%	1.280%
22	17.627	2433	2438	2442	rBV	43379	65266	3.01%	0.395%
23	18.339	2555	2559	2566	rBV2	153501	248363	11.45%	1.503%
24	18.404	2567	2570	2574	rVB2	39435	50045	2.31%	0.303%
25	18.551	2589	2595	2599	rBV3	41800	82888	3.82%	0.502%
26	18.845	2641	2645	2649	rBV3	21698	31909	1.47%	0.193%
27	19.062	2679	2682	2685	rBV4	15544	22656	1.04%	0.137%
28	19.257	2710	2715	2719	rBV4	41382	75931	3.50%	0.459%
29	19.527	2755	2761	2768	rBV	276293	436607	20.12%	2.642%
30	19.598	2770	2773	2783	rVB4	56647	91251	4.21%	0.552%
31	19.851	2812	2816	2818	rBV2	61485	86845	4.00%	0.526%
32	19.886	2818	2822	2828	rVB	265879	367708	16.95%	2.225%
33	19.951	2830	2833	2839	rVB6	25915	44895	2.07%	0.272%
34	20.068	2848	2853	2858	rBV	1880396	2169534	100.00%	13.128%

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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

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35	21.492	3092	3095	3099	rBV	100008	105277	4.85%	0.637%
36	21.621	3111	3117	3121	rBV2	459995	747640	34.46%	4.524%
37	21.656	3121	3123	3128	rVB	118323	141250	6.51%	0.855%
38	23.950	3508	3513	3520	rBV	258303	482631	22.25%	2.920%

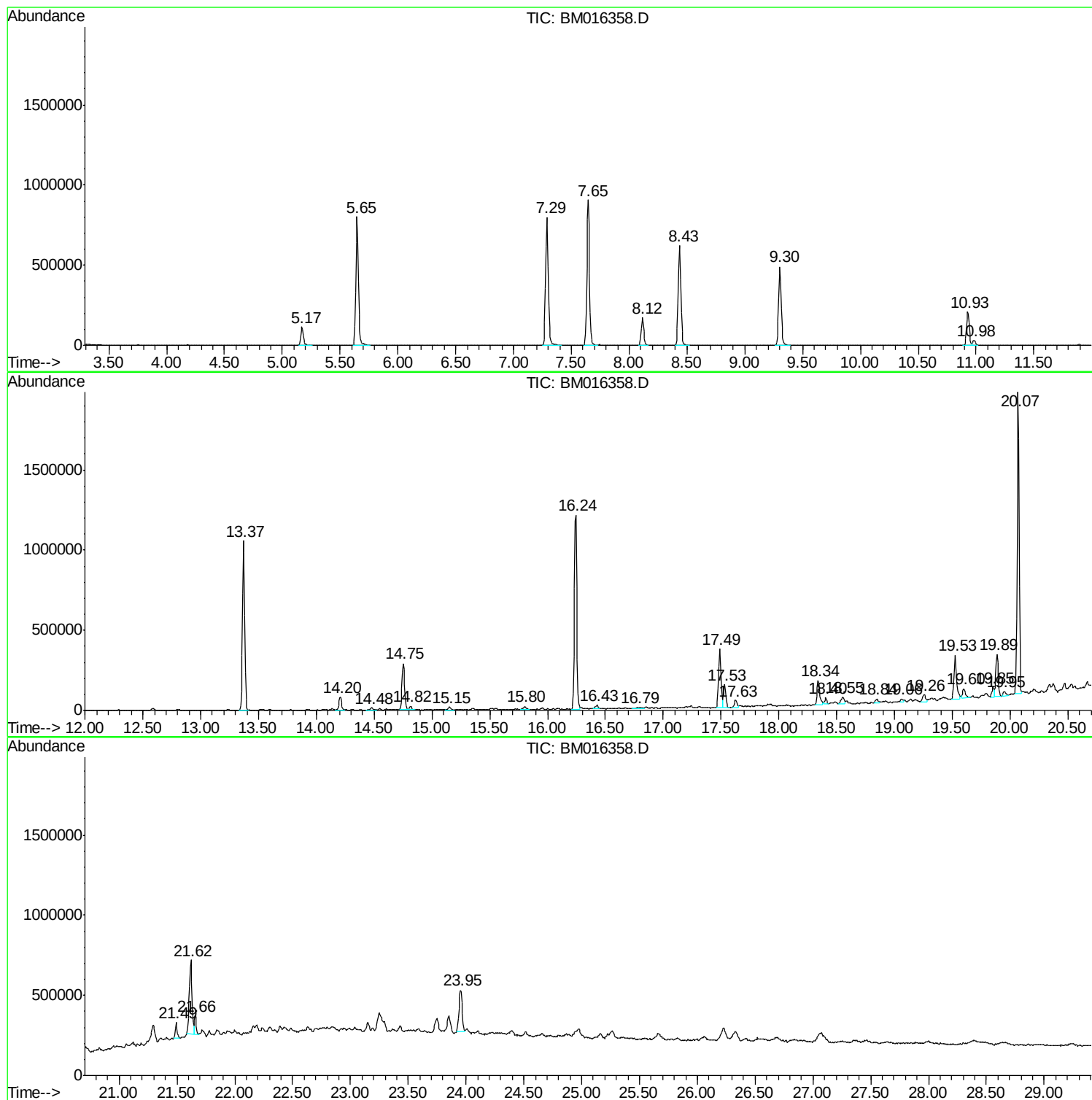
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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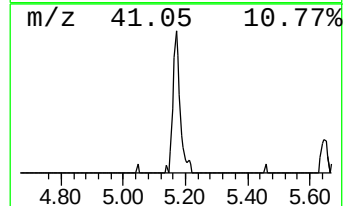
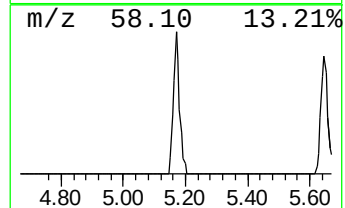
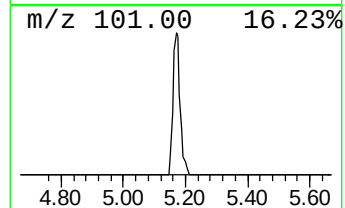
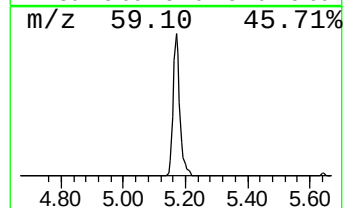
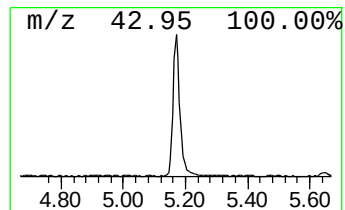
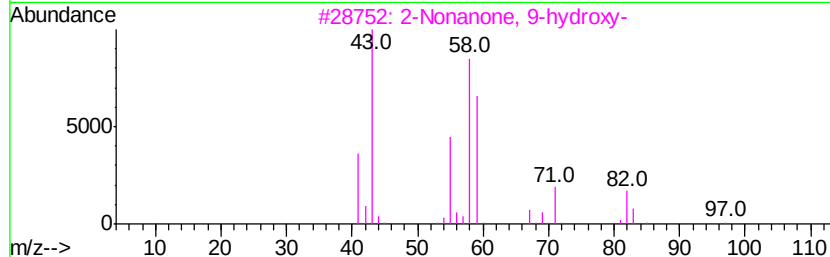
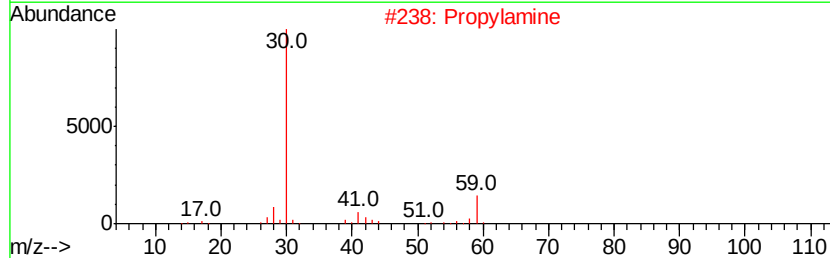
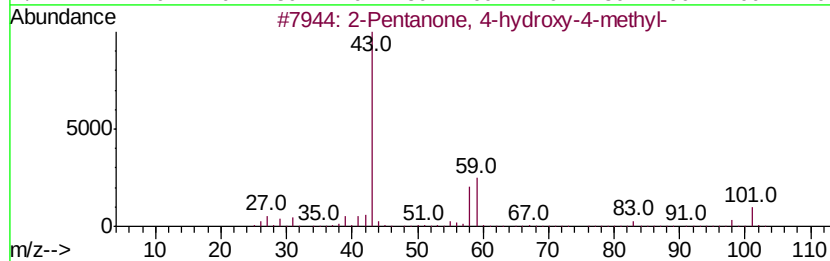
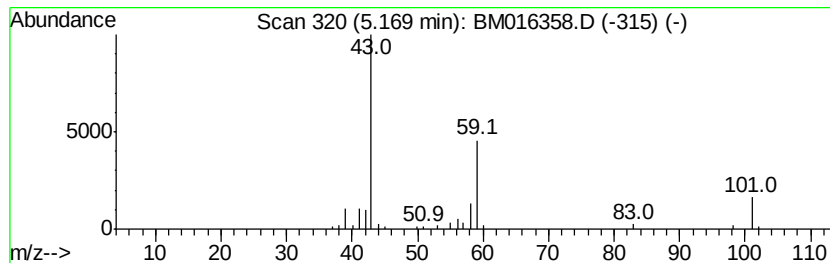
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	12.62 ng	173649	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propylamine	59	C3H9N	000107-10-8	42
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
5			Butane	58	C4H10	000106-97-8	27



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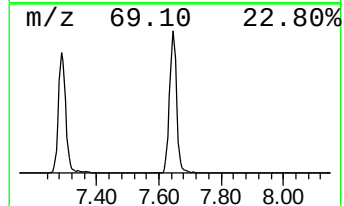
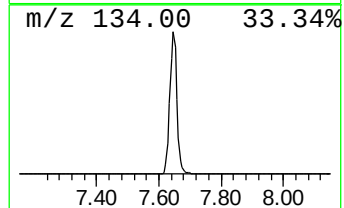
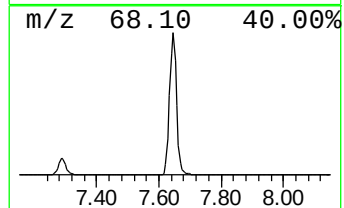
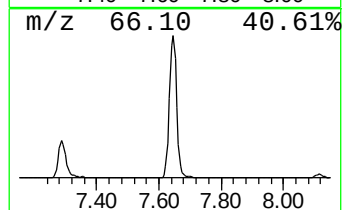
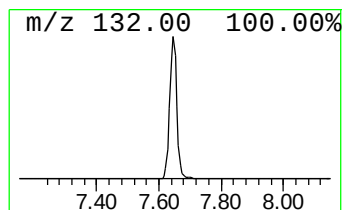
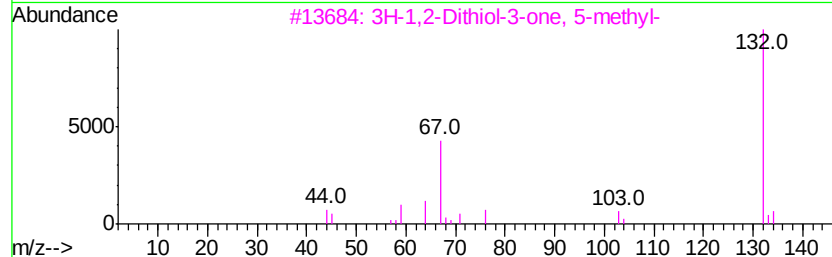
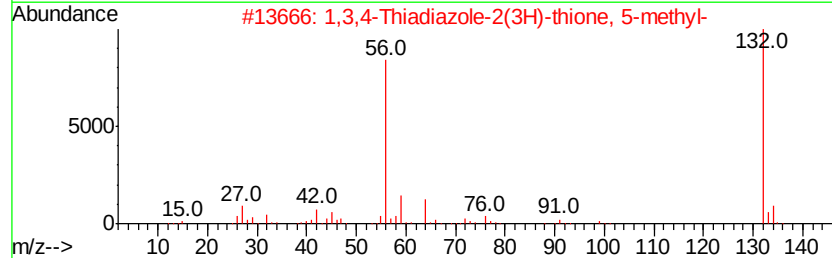
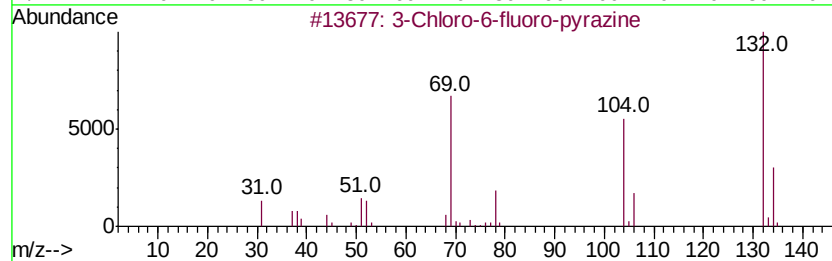
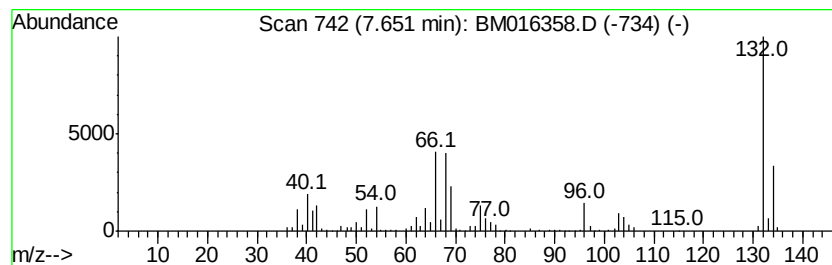
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Peak Number 2 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	103.56 ng	1424980	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12



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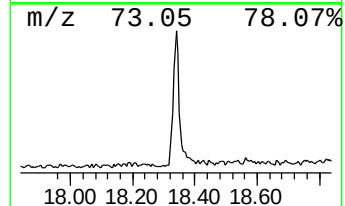
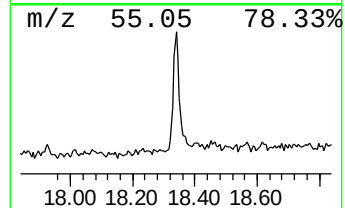
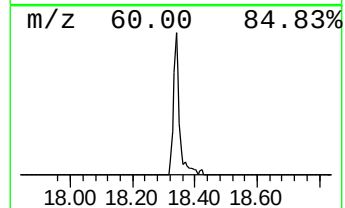
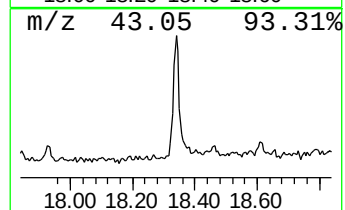
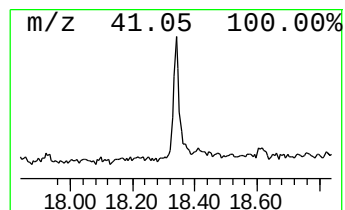
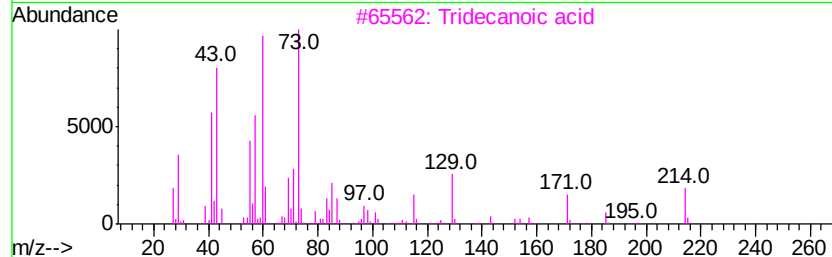
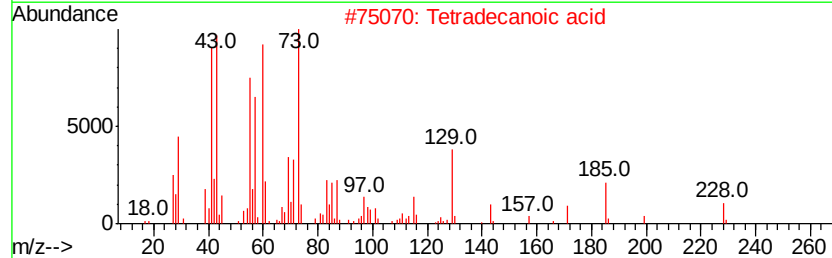
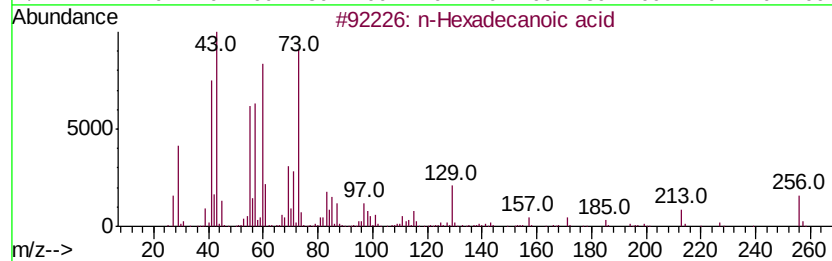
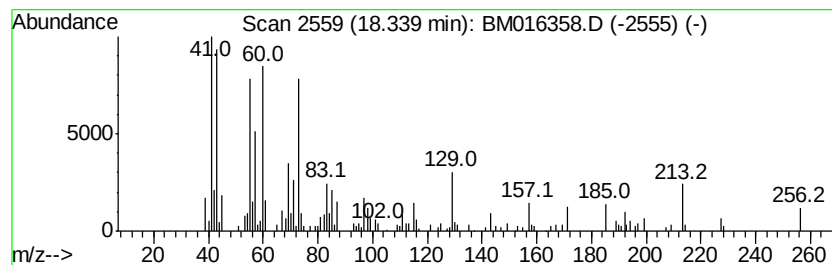
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.34	9.33 ng	248363	Phenanthrene-d10	17.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53



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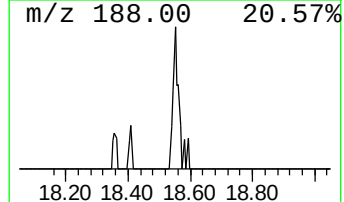
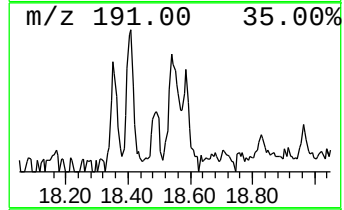
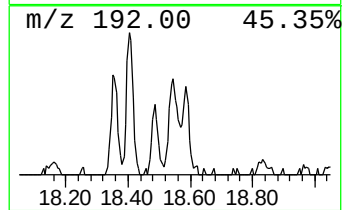
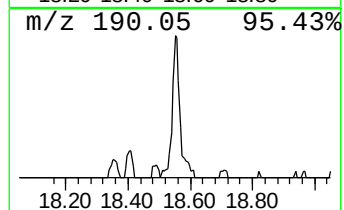
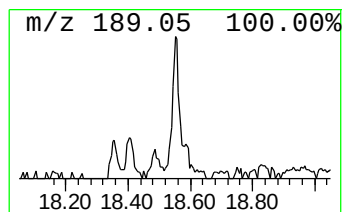
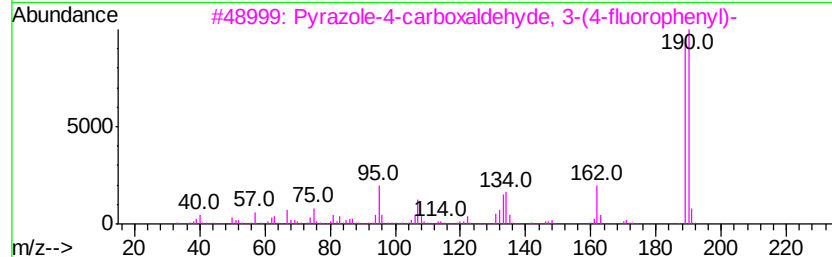
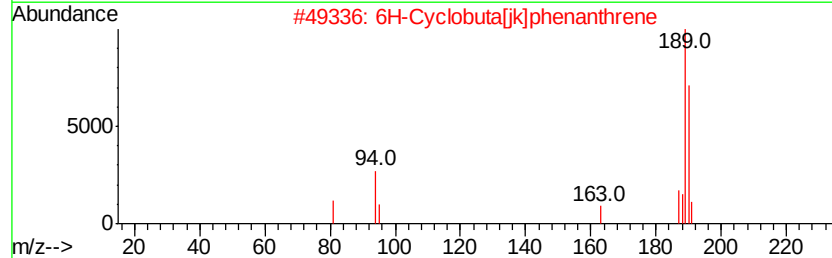
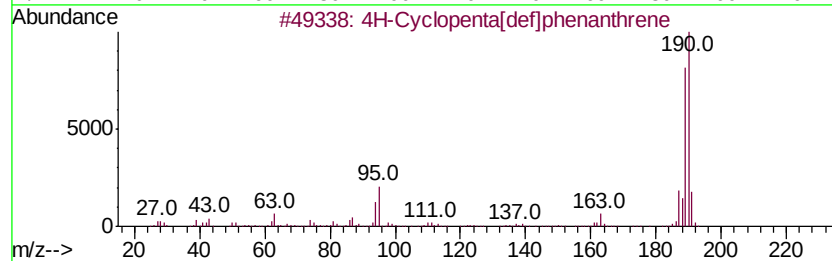
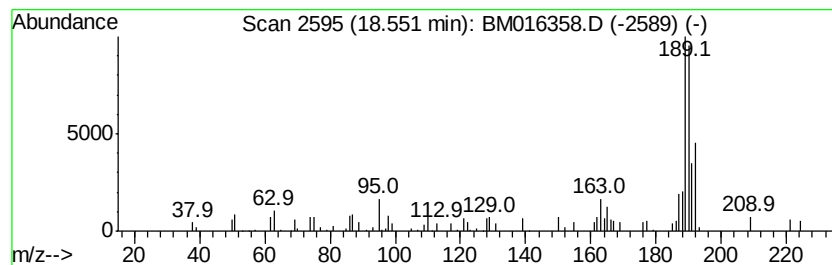
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.55	3.11 ng	82888	Phenanthrene-d10	17.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	59
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	37
4	3-(Trifluoromethoxy)benzaldehyde	190	C8H5F3O2	052771-21-8	37
5	4-(4-Chlorophenyl)pyridine	189	C11H8ClN	005957-96-0	27



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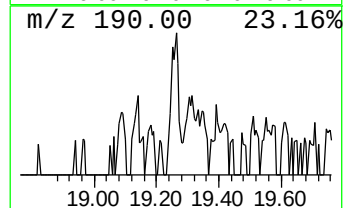
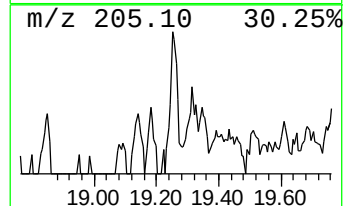
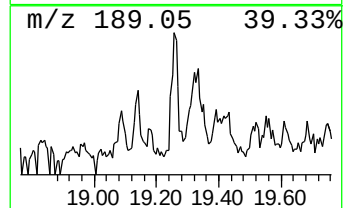
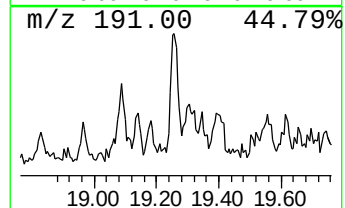
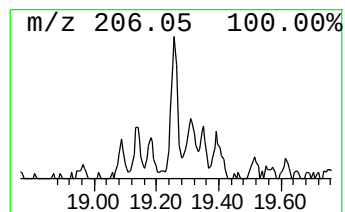
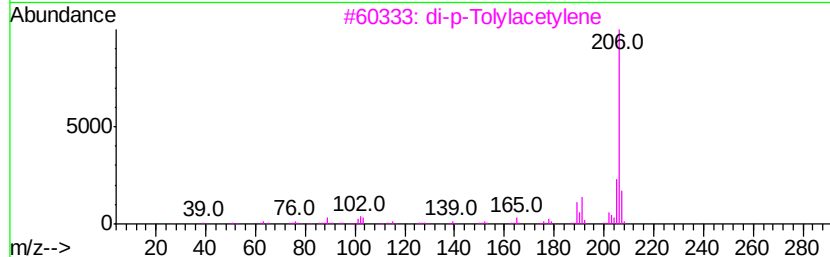
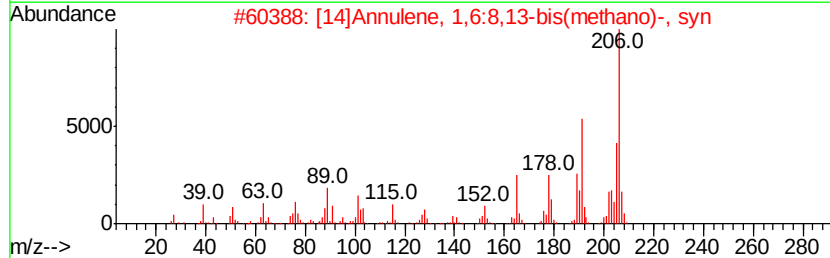
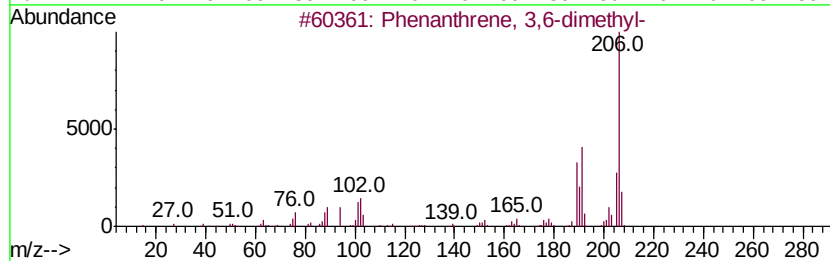
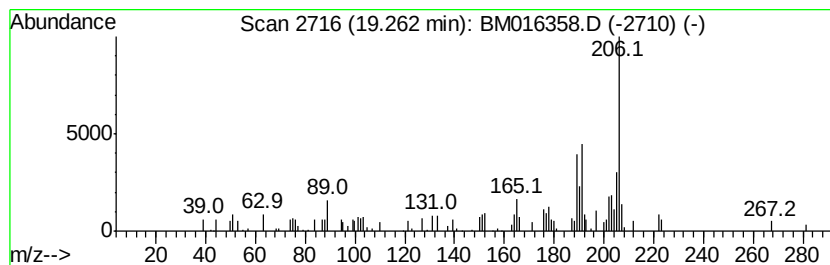
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenanthrene, 3,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.26	2.85 ng	75931	Phenanthrene-d10	17.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	91
2	[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	90
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	90
4	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	87
5	9,10-Dimethylantracene	206	C16H14	000781-43-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016358.D
Acq On : 14 Aug 2018 17:13
Operator : SJ/JU
Sample : J4427-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

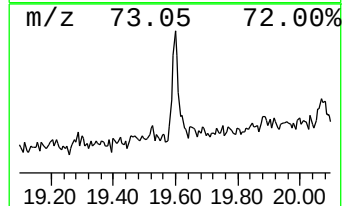
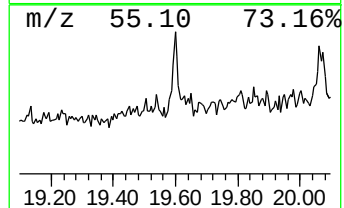
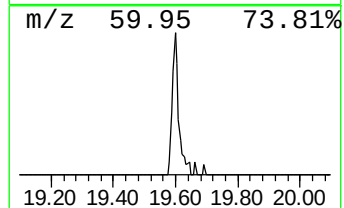
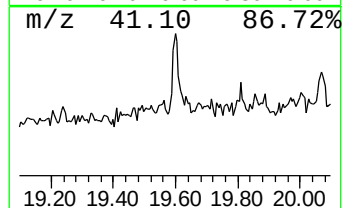
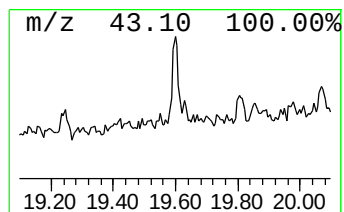
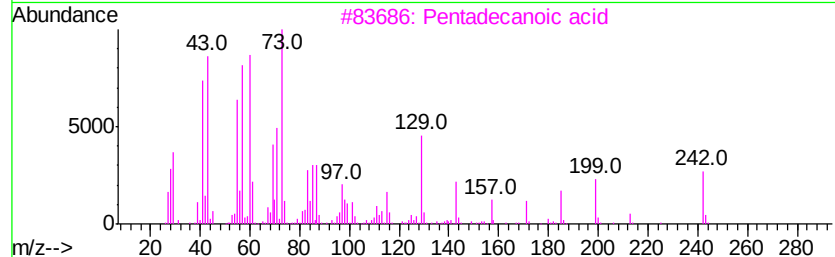
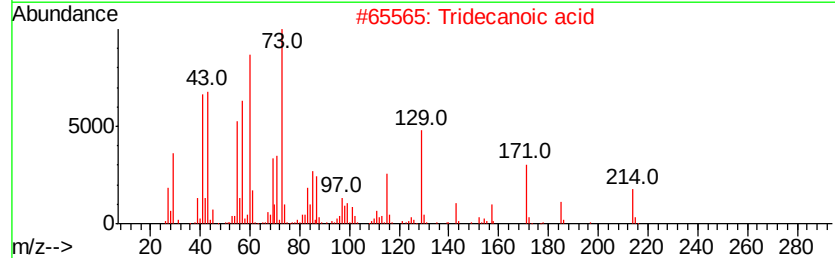
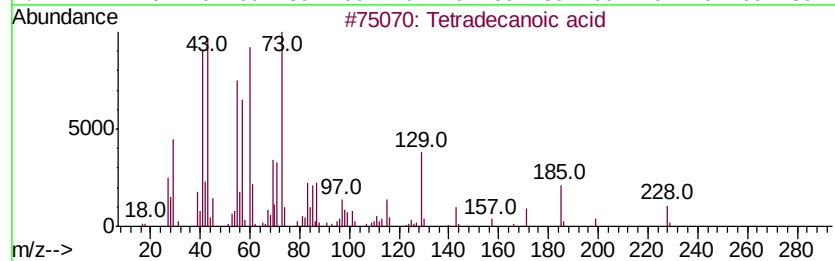
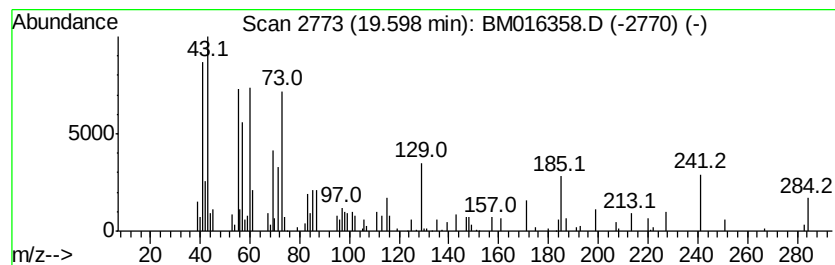
Instrument :
BNA_M
ClientSampleId :
RB47197

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 7 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.60	2.44 ng	91251	Chrysene-d12		21.62
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
2	Tridecanoic acid	214	C13H26O2	000638-53-9	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM081418\
Data File : BM016358.D
Acq On : 14 Aug 2018 17:13
Operator : SJ/JU
Sample : J4427-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RB47197

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	12.6	ng	173649	1	8.12	275195	20.0
unknown7.65	7.65	103.6	ng	1424980	1	8.12	275195	20.0
n-Hexadecanoic acid	18.34	9.3	ng	248363	4	17.49	532560	20.0
4H-Cyclopenta[def...	18.55	3.1	ng	82888	4	17.49	532560	20.0
Phenanthrene, 3,6...	19.26	2.9	ng	75931	4	17.49	532560	20.0
Tetradecanoic acid	19.60	2.4	ng	91251	5	21.62	747640	20.0