

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
 Data File : BM039102.D
 Acq On : 22 Mar 2023 21:22
 Operator : CG/JU
 Sample : 02020-11
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-2

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-BM030823.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039102.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	295	300	308	rBV	1831105	2508970	28.37%	3.124%
2	5.522	373	380	390	rBV	4261280	5964217	67.43%	7.427%
3	6.640	564	570	579	rVB	145756	229016	2.59%	0.285%
4	7.128	643	653	668	rBV	3990971	6138258	69.40%	7.644%
5	7.398	694	699	710	rVB	54944	95889	1.08%	0.119%
6	7.963	788	795	803	rBV	1041259	1618111	18.29%	2.015%
7	9.134	986	994	1005	rBV	2354862	3776762	42.70%	4.703%
8	10.010	1136	1143	1151	rBV	66577	173808	1.97%	0.216%
9	10.775	1266	1273	1280	rBV	1263661	2123011	24.00%	2.644%
10	13.233	1684	1691	1701	rBV	5126040	7413311	83.82%	9.232%
11	13.486	1729	1734	1739	rBV	117199	163571	1.85%	0.204%
12	13.704	1766	1771	1777	rBV	79584	144049	1.63%	0.179%
13	13.927	1804	1809	1814	rVB3	85271	127582	1.44%	0.159%
14	14.016	1814	1824	1829	rBV3	89430	141981	1.61%	0.177%
15	14.445	1890	1897	1902	rBV4	79401	142301	1.61%	0.177%
16	14.563	1909	1917	1920	rBV	463360	661716	7.48%	0.824%
17	14.604	1920	1924	1931	rVV	1774765	2516831	28.46%	3.134%
18	14.674	1931	1936	1945	rVB4	108606	227538	2.57%	0.283%
19	14.851	1960	1966	1974	rBV2	382643	733997	8.30%	0.914%
20	14.921	1974	1978	1984	rVB2	88274	155013	1.75%	0.193%
21	15.004	1987	1992	2000	rBV2	50434	122343	1.38%	0.152%
22	15.933	2145	2150	2151	rBV3	108864	141228	1.60%	0.176%
23	15.963	2151	2155	2162	rVB	232276	391573	4.43%	0.488%
24	16.092	2169	2177	2186	rVB	3716542	5701153	64.46%	7.100%
25	16.245	2198	2203	2208	rVB7	53522	92369	1.04%	0.115%
26	16.486	2239	2244	2250	rVB3	50714	91056	1.03%	0.113%
27	16.745	2283	2288	2295	rBV4	79016	145547	1.65%	0.181%
28	17.168	2356	2360	2368	rVB	50366	90078	1.02%	0.112%
29	17.351	2385	2391	2394	rBV	1961719	2762647	31.23%	3.440%
30	17.392	2394	2398	2403	rVB	802852	1069900	12.10%	1.332%
31	17.751	2456	2459	2465	rVB	64354	93729	1.06%	0.117%
32	18.186	2529	2533	2536	rBV3	77441	115557	1.31%	0.144%
33	18.245	2537	2543	2553	rVV2	1018717	1752746	19.82%	2.183%
34	18.421	2568	2573	2577	rBV3	93663	153001	1.73%	0.191%
35	18.768	2627	2632	2641	rVB2	172021	249535	2.82%	0.311%
36	19.280	2716	2719	2724	rVB2	75080	101376	1.15%	0.126%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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37	19.403	2732	2740	2747	rBV	1076949	1633574	18.47%	2.034%
38	19.515	2755	2759	2769	rBV2	375831	633994	7.17%	0.790%
39	19.733	2793	2796	2797	rBV	95059	103165	1.17%	0.128%
40	19.762	2797	2801	2810	rVB	816212	1232897	13.94%	1.535%
41	19.968	2830	2836	2845	rBV	7363381	8844844	100.00%	11.015%
42	20.562	2933	2937	2941	rBV	636692	766161	8.66%	0.954%
43	20.815	2976	2980	2985	rBV	1854374	2048525	23.16%	2.551%
44	21.074	3020	3024	3029	rBV	2461059	2611023	29.52%	3.252%
45	21.233	3047	3051	3058	rVB2	788919	1055177	11.93%	1.314%
46	21.527	3095	3101	3105	rBV	2598059	3759899	42.51%	4.682%
47	21.562	3105	3107	3113	rVB	389380	453653	5.13%	0.565%
48	22.168	3203	3210	3216	rBV3	356499	823172	9.31%	1.025%
49	23.209	3382	3387	3392	rBV2	1526080	2571187	29.07%	3.202%
50	23.956	3508	3514	3521	rVB2	1663245	3243722	36.67%	4.039%
51	24.574	3614	3619	3628	rVB	1158074	2389841	27.02%	2.976%

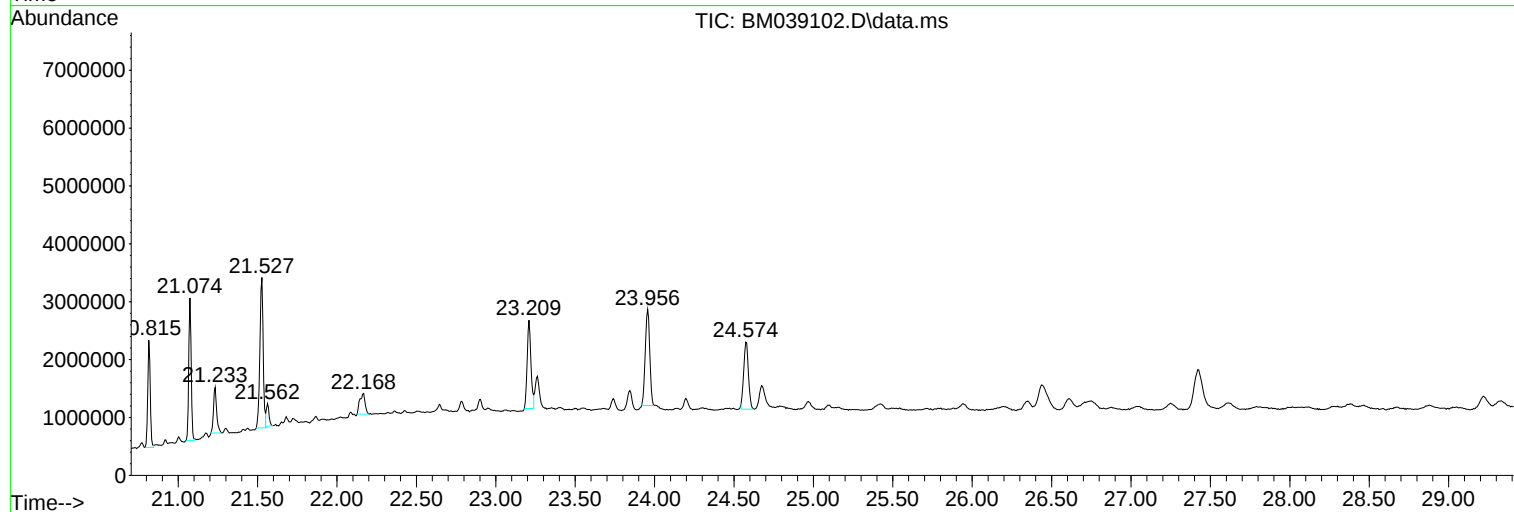
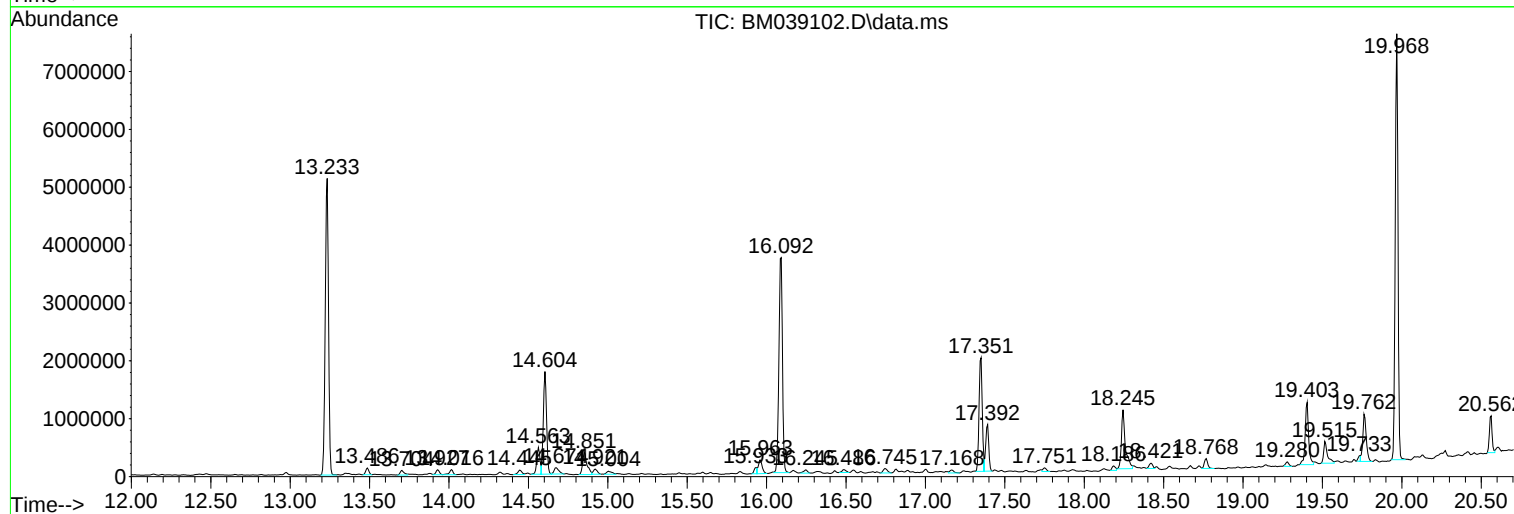
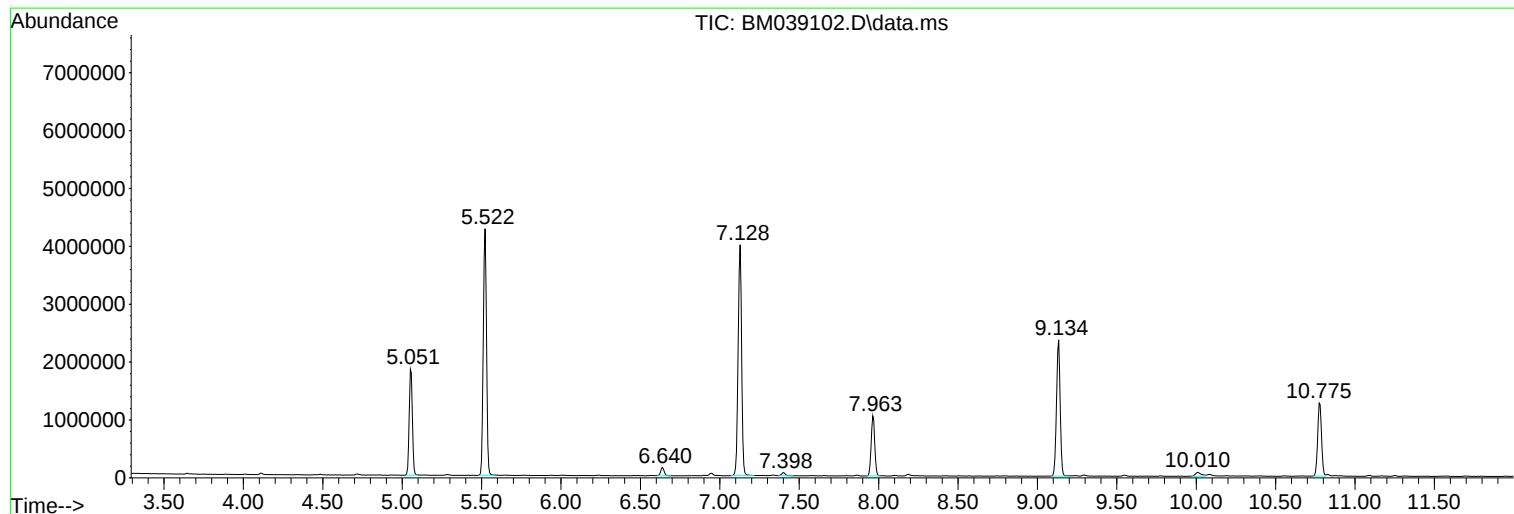
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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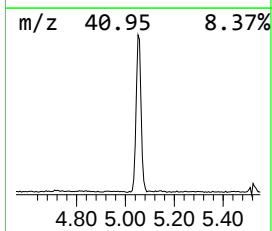
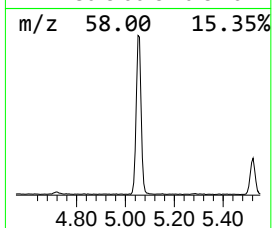
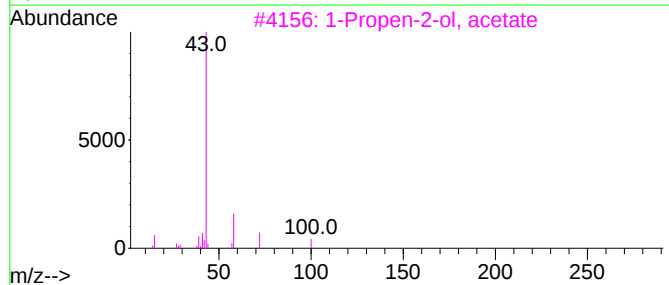
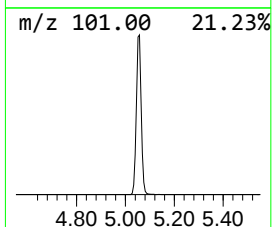
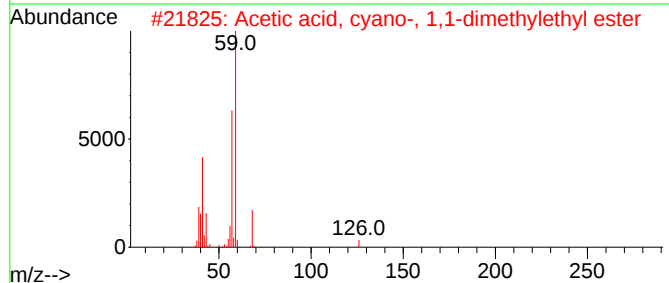
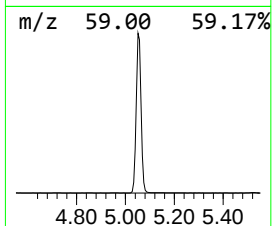
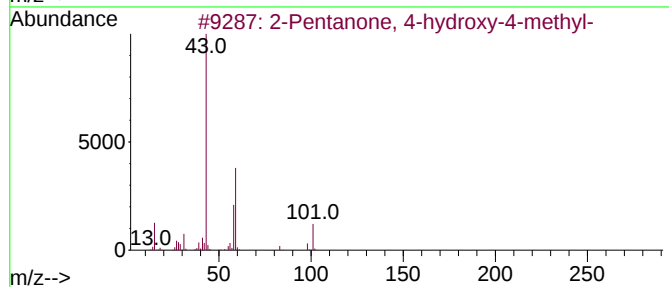
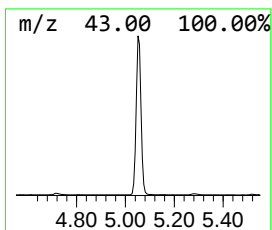
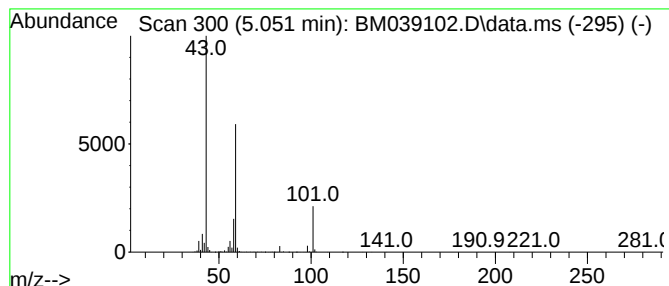
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	31.01 ng	2508970	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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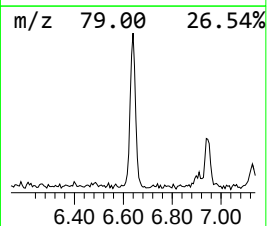
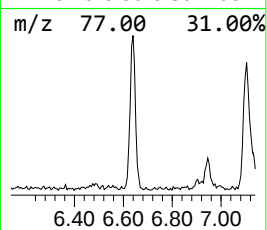
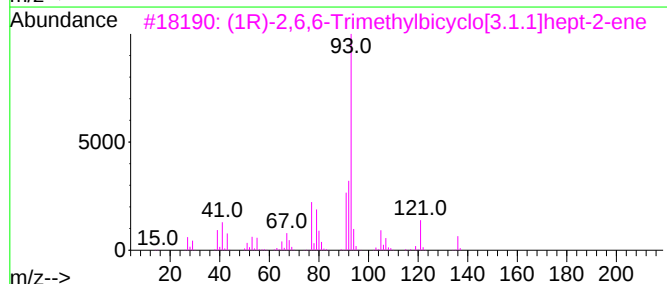
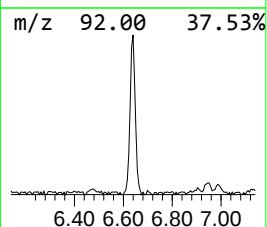
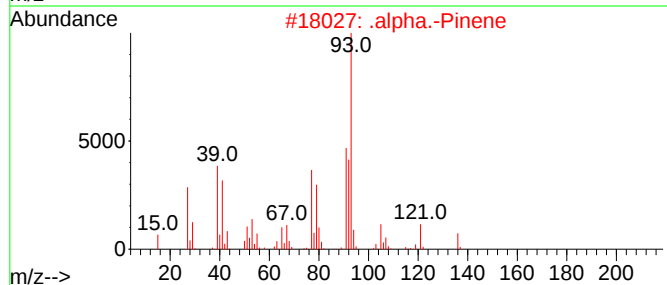
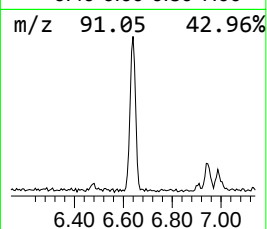
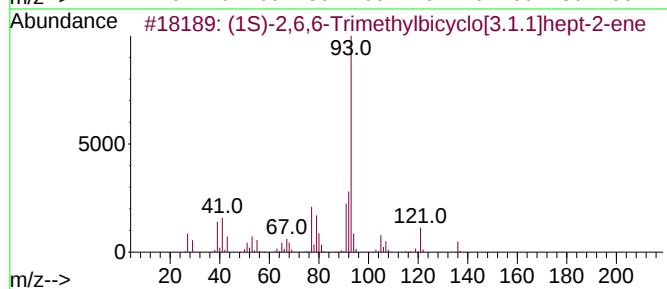
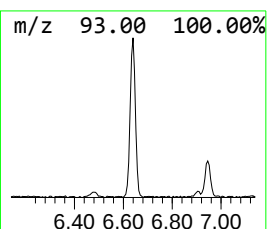
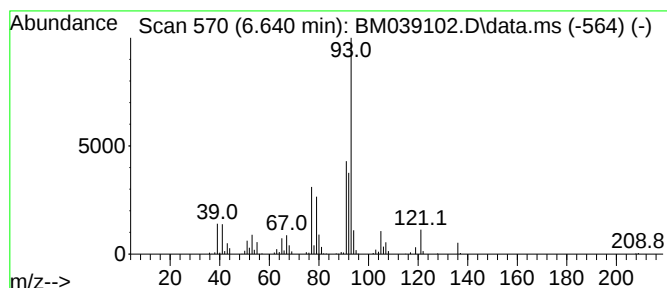
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.640	2.83 ng	229016	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	95		
2	.alpha.-Pinene	136	C10H16	000080-56-8	95		
3	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	93		
4	3-Carene	136	C10H16	013466-78-9	91		
5	(+)-3-Carene	136	C10H16	000498-15-7	91		



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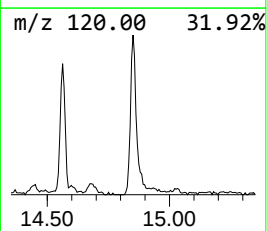
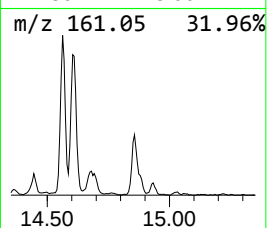
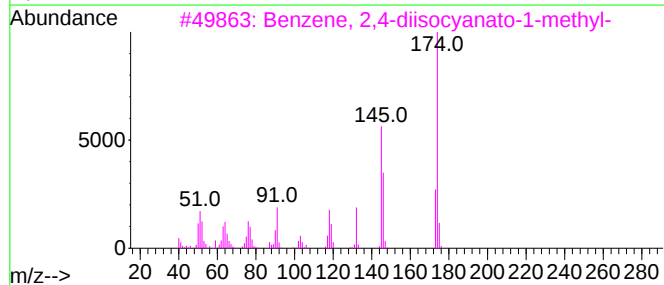
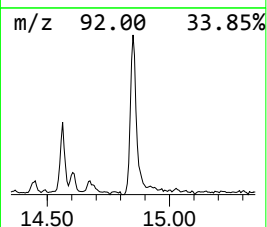
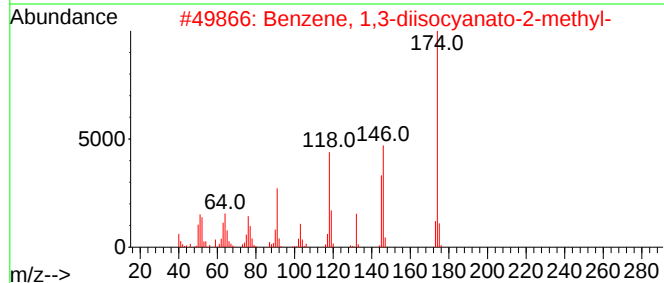
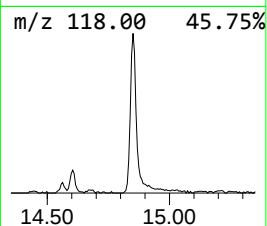
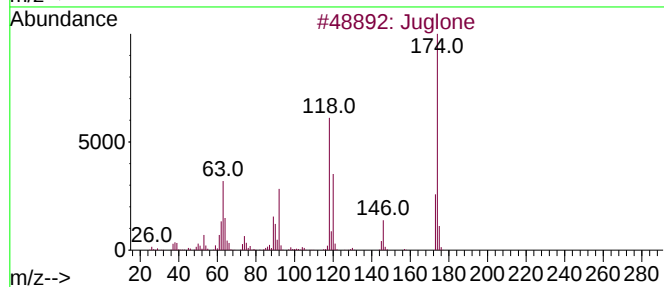
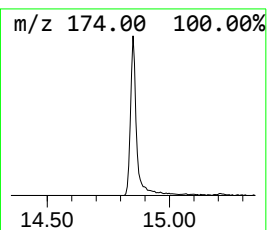
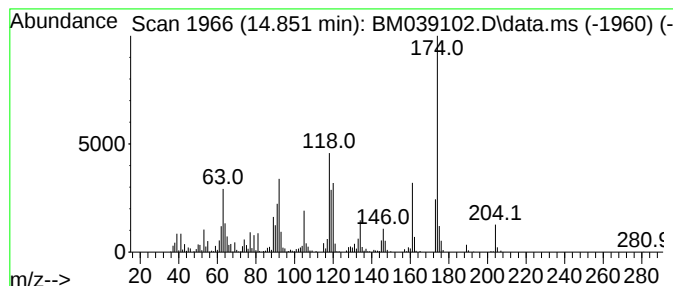
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Peak Number 3 Juglone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	5.83 ng	733997	Acenaphthene-d10	14.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Juglone	174	C10H6O3	000481-39-0	98
2			Benzene, 1,3-diisocyanato-2-methyl-	174	C9H6N2O2	000091-08-7	46
3			Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	41
4			4-(4-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-19-4	30
5			Benzaldehyde, 2,6-difluoro-3,4-d...	174	C7H4F2O3	152434-98-5	27



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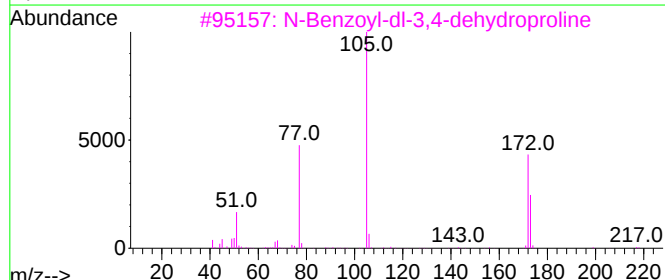
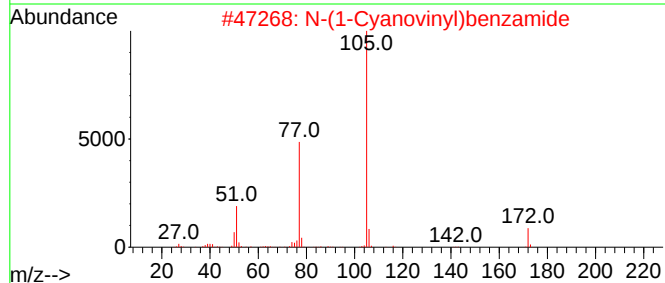
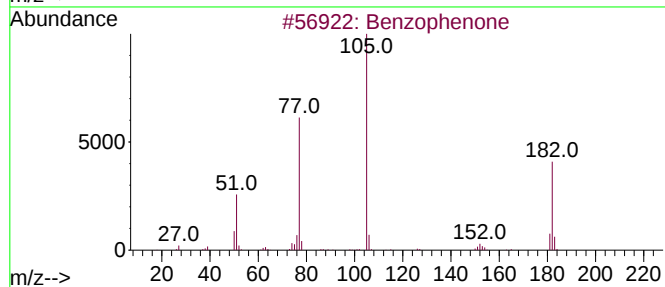
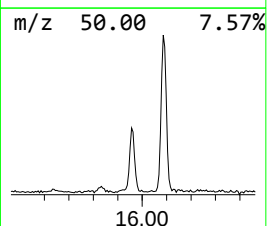
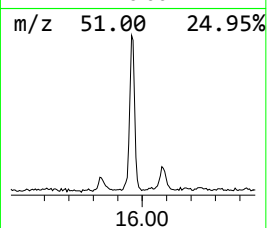
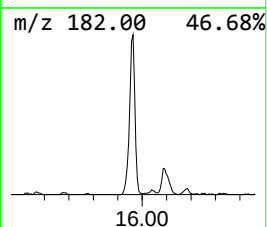
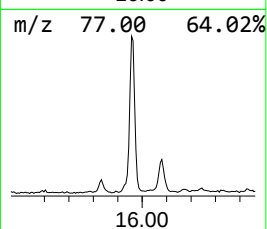
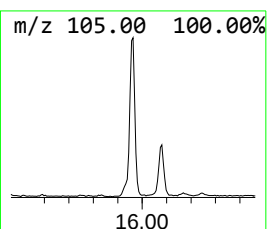
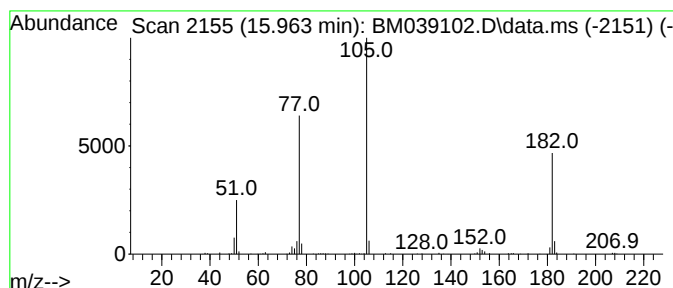
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Peak Number 4 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.963	3.11 ng	391573	Acenaphthene-d10	14.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47
3			N-Benzoyl-dl-3,4-dehydroproline	217	C12H11NO3	093001-94-6	47
4			1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
5			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	47



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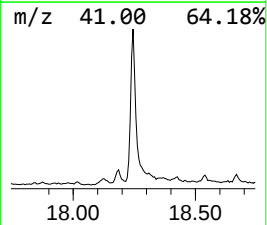
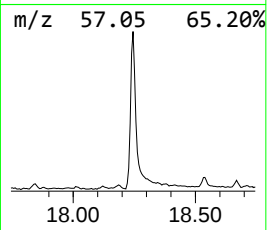
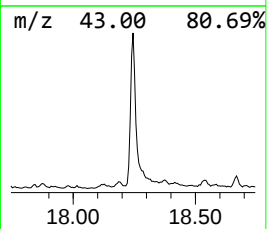
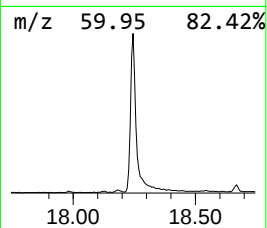
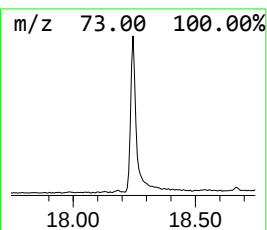
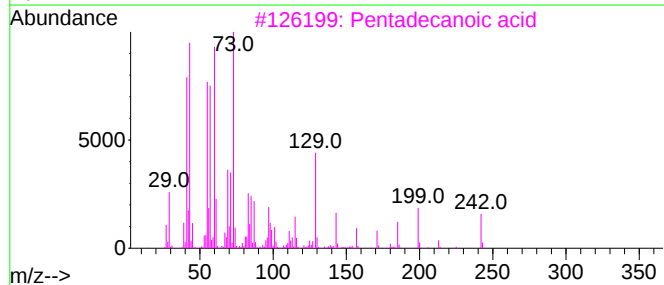
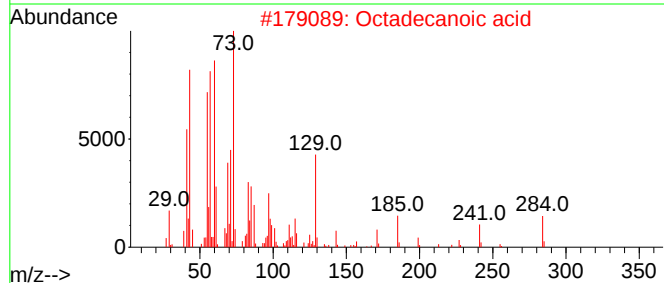
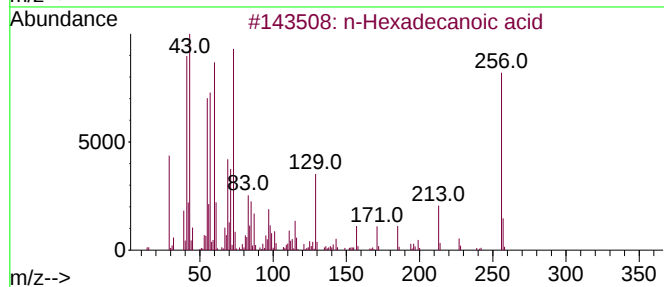
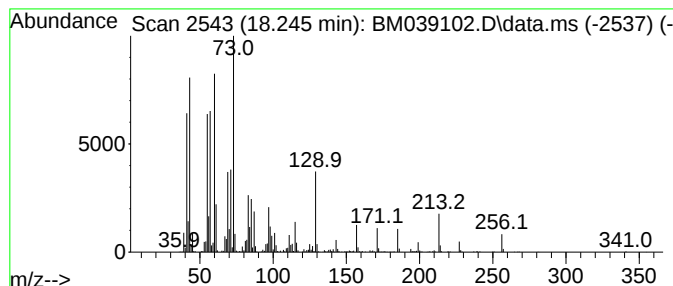
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.245	12.69 ng	1752750	Phenanthrene-d10	17.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5	Tridecanoic acid	214	C13H26O2	000638-53-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039102.D
Acq On : 22 Mar 2023 21:22
Operator : CG/JU
Sample : 02020-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

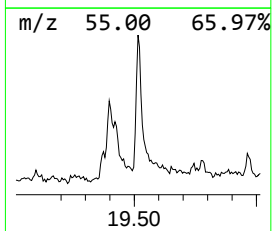
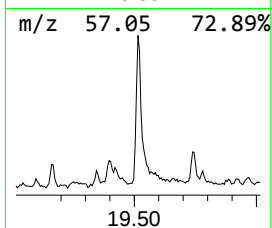
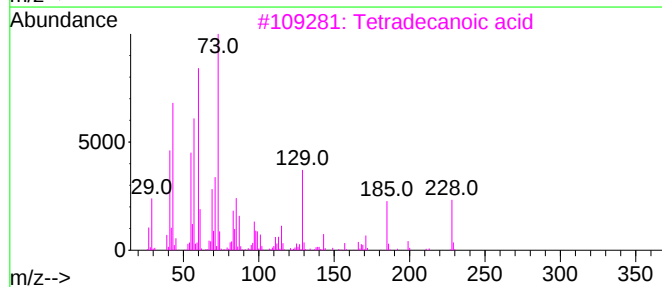
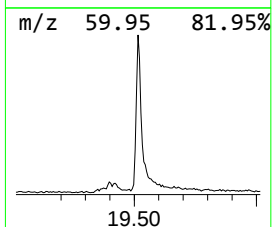
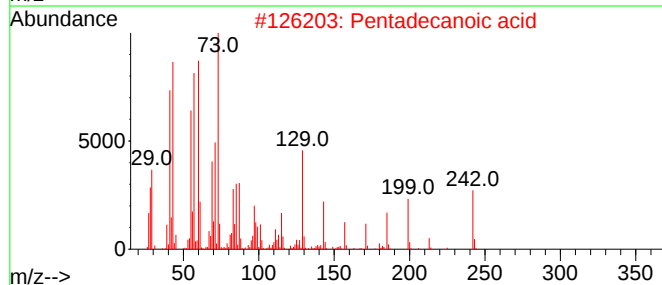
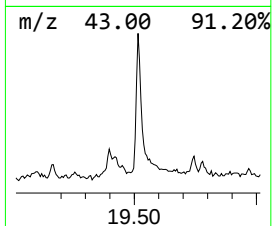
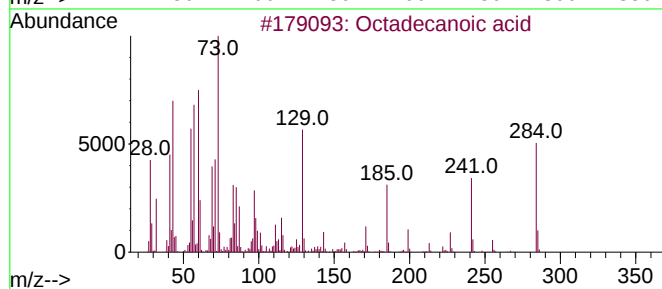
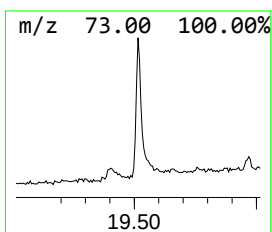
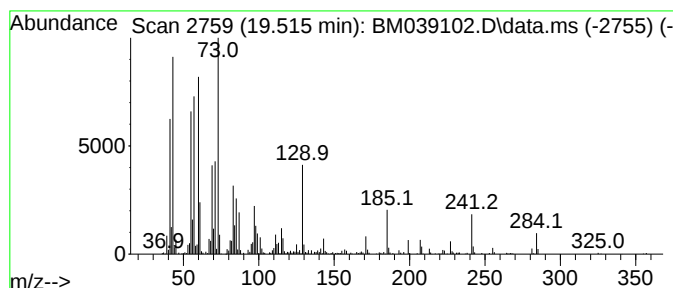
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.515	3.37 ng	633994	Chrysene-d12	21.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039102.D
Acq On : 22 Mar 2023 21:22
Operator : CG/JU
Sample : 02020-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP-2

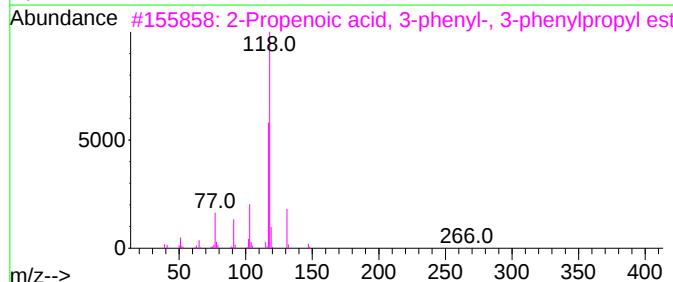
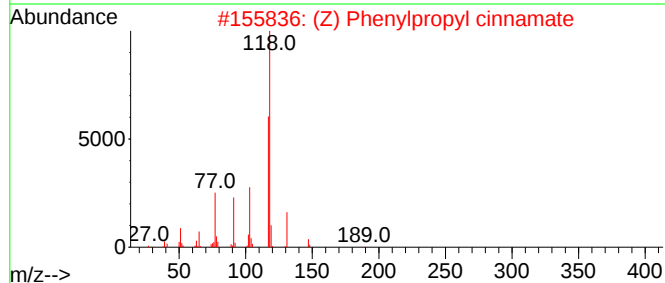
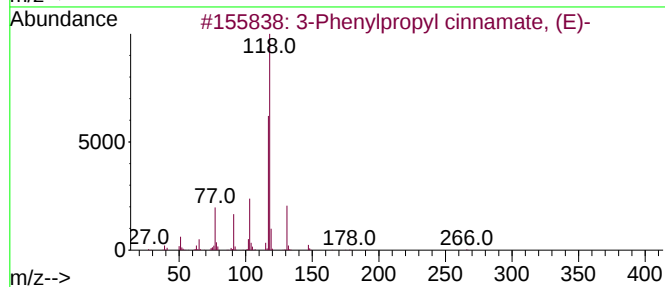
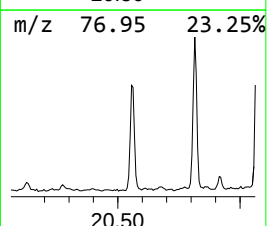
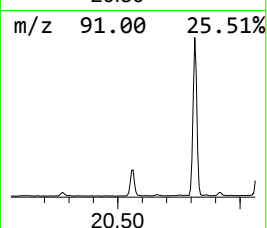
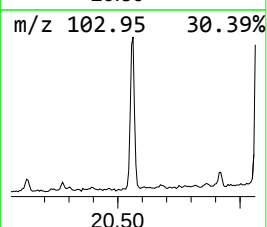
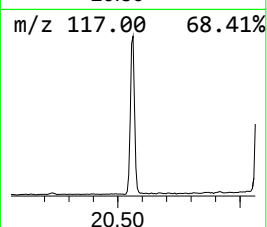
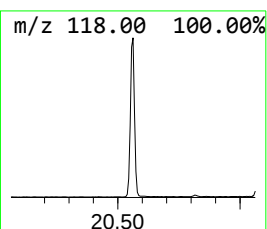
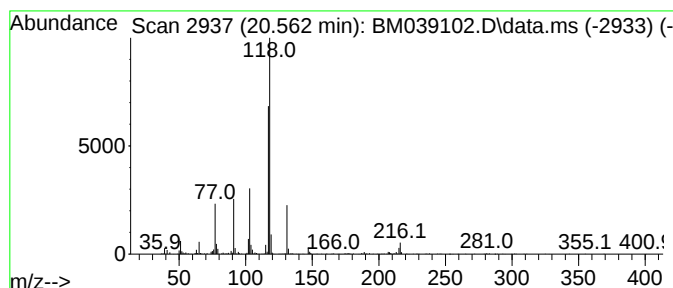
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 3-Phenylpropyl cinnamate, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.562	4.08 ng	766161	Chrysene-d12	21.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Phenylpropyl cinnamate, (E)-	266	C18H18O2	290311-72-7	91
2		(Z) Phenylpropyl cinnamate	266	C18H18O2	1000414-29-1	80
3		2-Propenoic acid, 3-phenyl-, 3-p...	266	C18H18O2	000122-68-9	80
4		.alpha.-Methylstyrene	118	C9H10	000098-83-9	64
5		Acetic acid, chloro-, 3-phenylpr...	212	C11H13ClO2	064046-48-6	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039102.D
Acq On : 22 Mar 2023 21:22
Operator : CG/JU
Sample : 02020-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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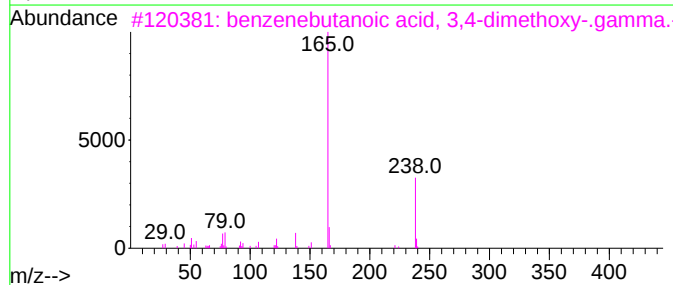
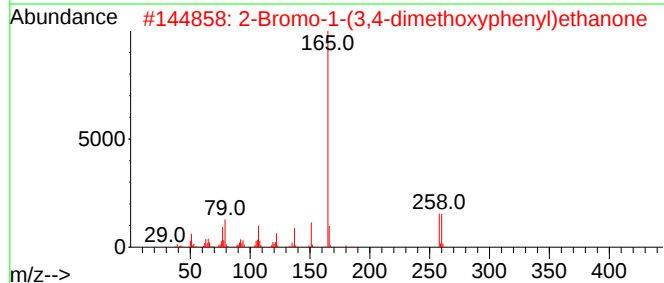
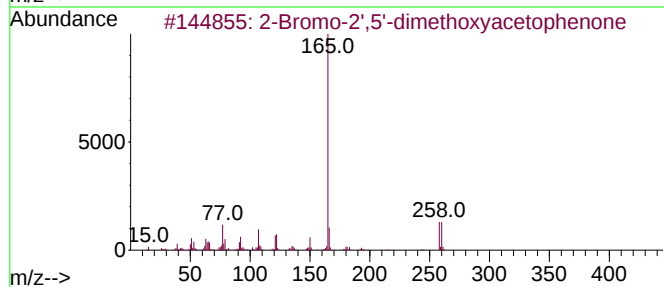
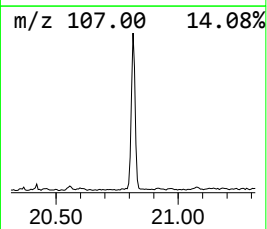
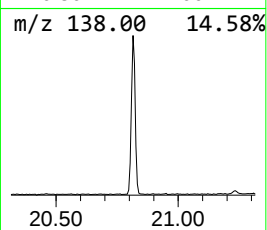
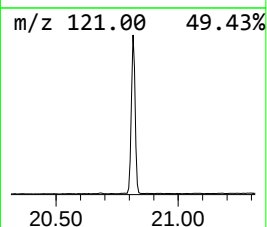
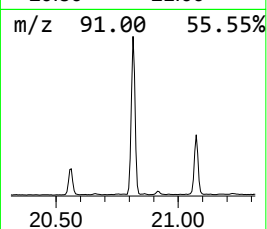
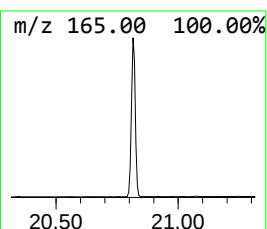
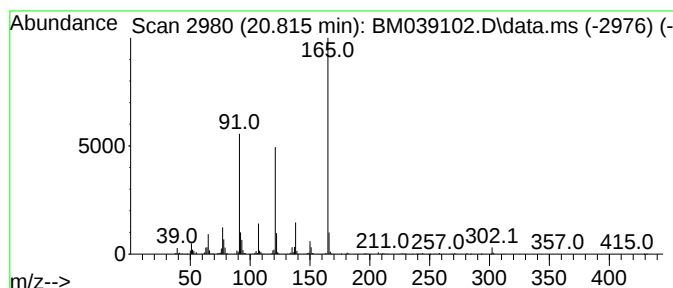
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 2-Bromo-2',5'-dimethoxyacet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.815	10.90 ng	2048530	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Bromo-2',5'-dimethoxyacetophenone	258	C10H11BrO3	001204-21-3	64
2			2-Bromo-1-(3,4-dimethoxyphenyl)e...	258	C10H11BrO3	001835-02-5	59
3			benzenebutanoic acid, 3,4-dimeth...	238	C12H14O5	1000401-14-9	59
4			Ethanone, 2-bromo-1-(2,4-dimetho...	258	C10H11BrO3	060965-26-6	59
5			1-(2,4-Dihydroxyphenyl)-2-(3,5-d...	330	C19H22O5	1000481-00-1	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039102.D
Acq On : 22 Mar 2023 21:22
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Instrument :
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ClientSampleId :
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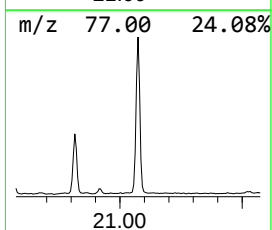
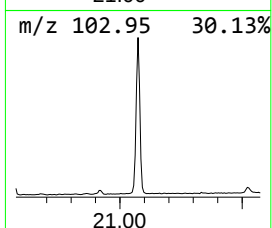
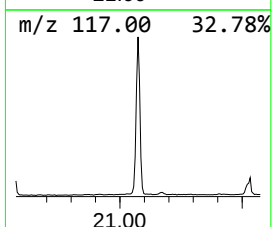
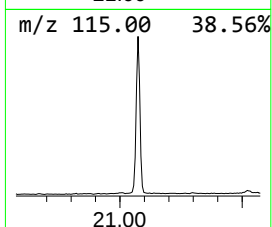
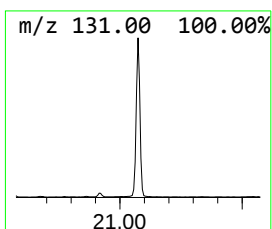
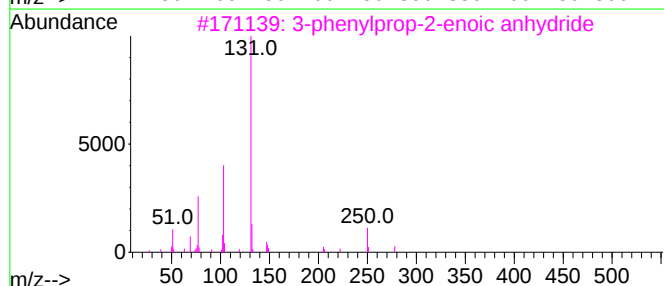
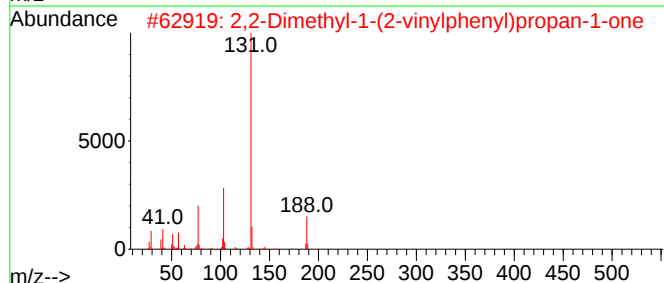
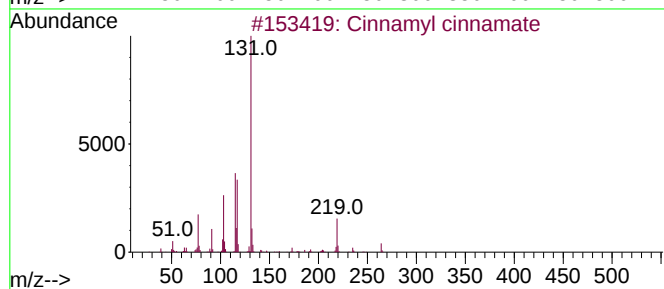
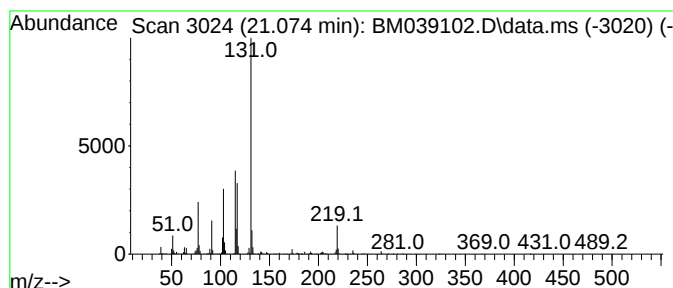
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Cinnamyl cinnamate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	13.89 ng	2611020	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	49
3			3-phenylprop-2-enoic anhydride	278	C18H14O3	1010401-87-5	47
4			1-Penten-3-one, 4-methyl-1-phenyl-	174	C12H14O	003160-32-5	47
5			1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039102.D
Acq On : 22 Mar 2023 21:22
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Sample : 02020-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

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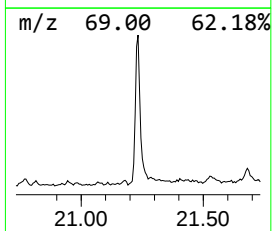
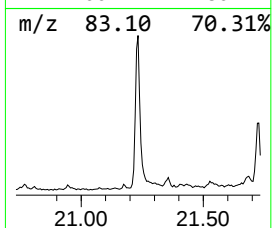
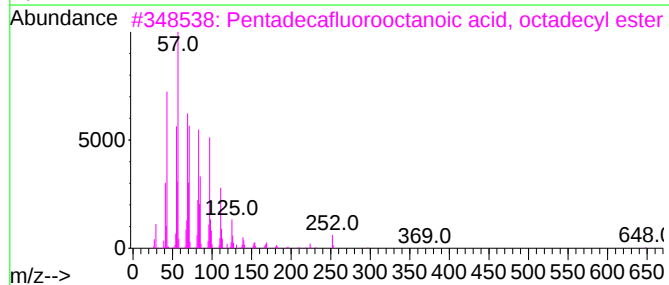
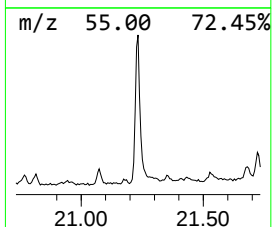
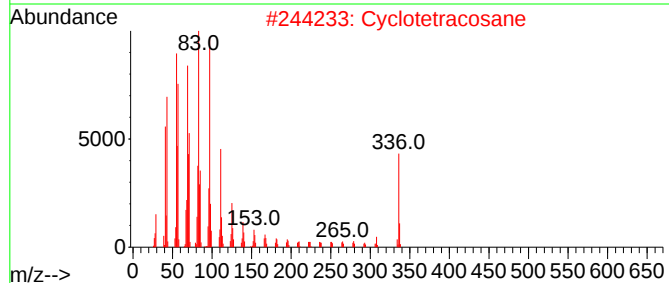
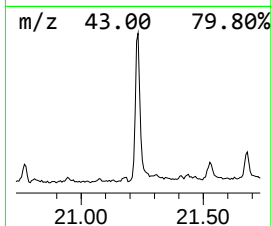
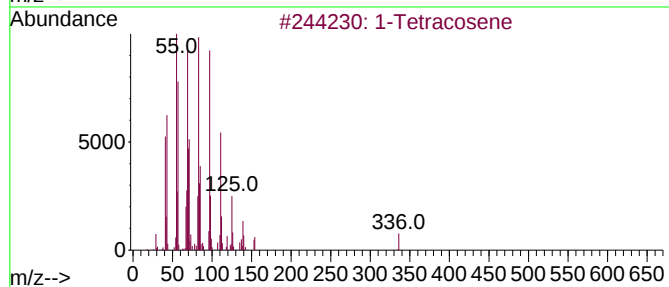
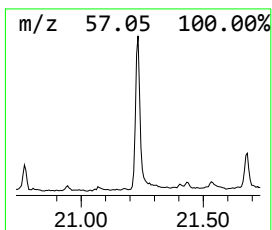
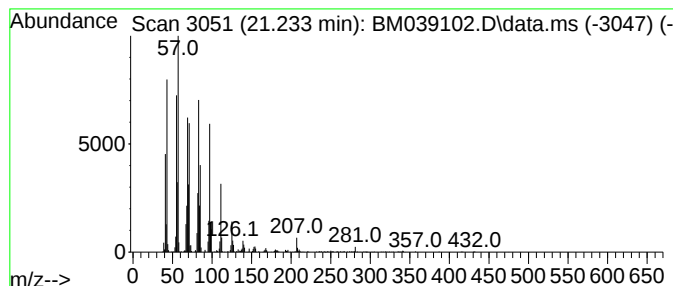
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Tetracosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	5.61 ng	1055180	Chrysene-d12	21.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Tetracosene	336	C24H48	010192-32-2	97
2		Cyclotetracosane	336	C24H48	000297-03-0	97
3		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4		Cyclopentadecane	210	C15H30	000295-48-7	92
5		1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039102.D
Acq On : 22 Mar 2023 21:22
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ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId :
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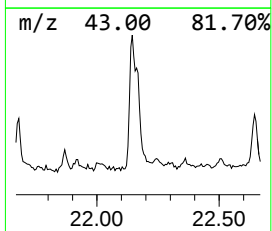
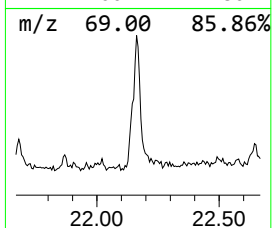
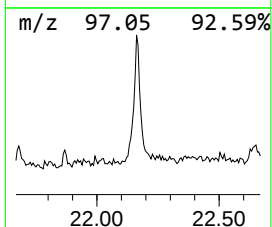
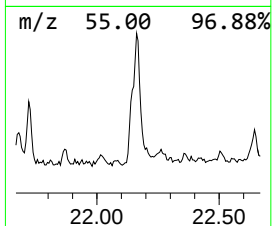
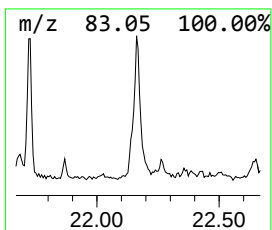
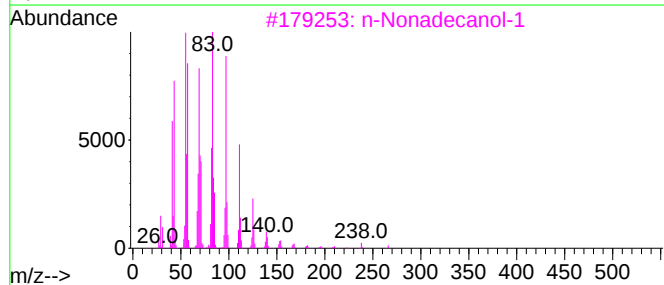
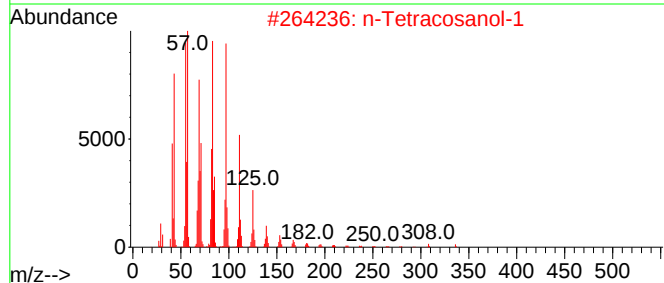
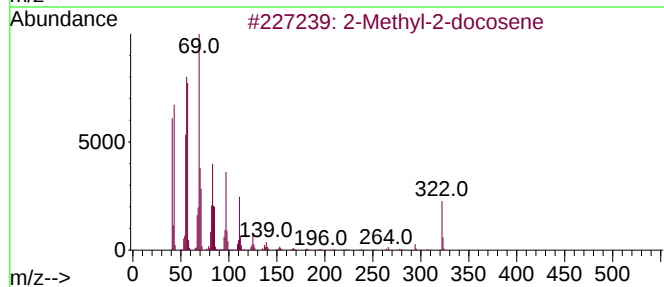
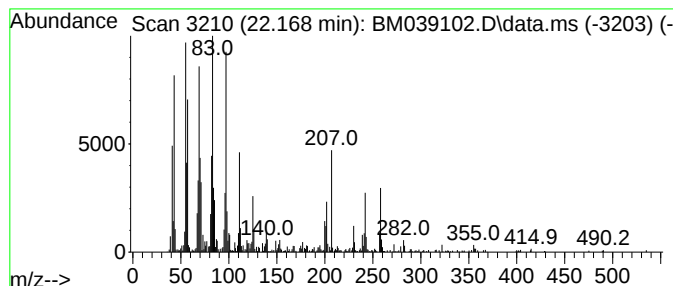
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2-Methyl-2-docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.168	4.38 ng	823172	Chrysene-d12	21.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methyl-2-docosene	322	C23H46	1000131-16-9	87
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	86
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	86
4		1-Heneicosanol	312	C21H44O	015594-90-8	86
5		9-Tricosene, (Z)-	322	C23H46	027519-02-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039102.D
Acq On : 22 Mar 2023 21:22
Operator : CG/JU
Sample : 02020-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-2

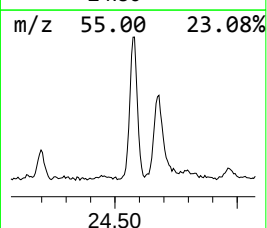
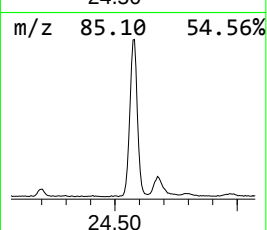
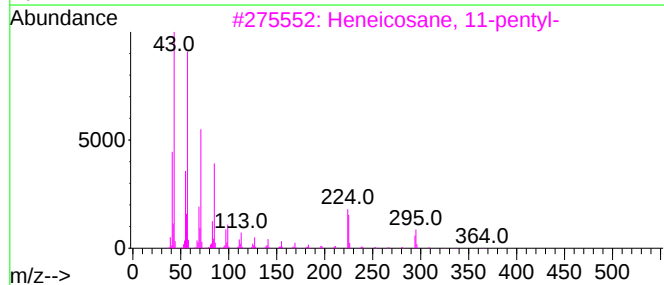
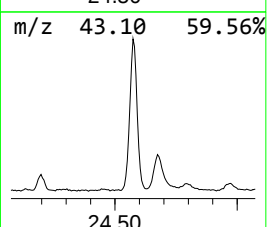
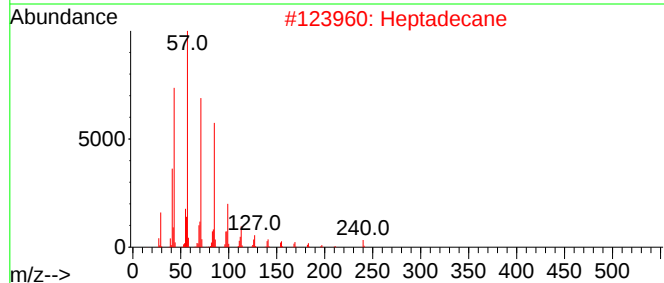
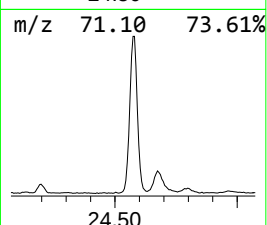
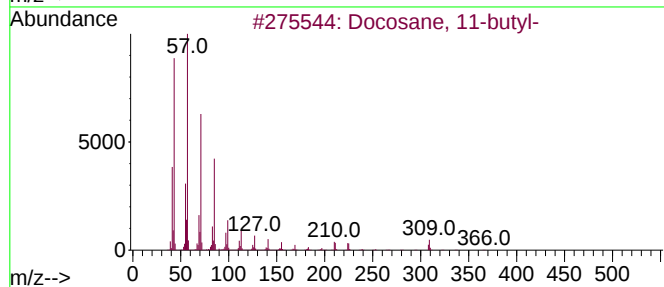
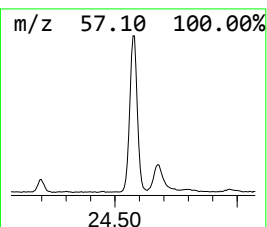
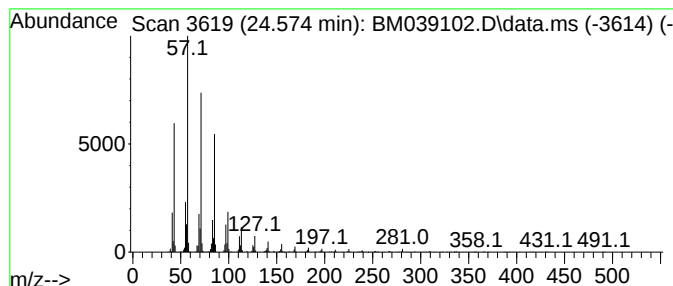
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Docosane, 11-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.574	14.74 ng	2389840	Perylene-d12	23.956

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosane, 11-butyl-	366	C26H54	013475-76-8	95
2		Heptadecane	240	C17H36	000629-78-7	94
3		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	94
4		Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039102.D
Acq On : 22 Mar 2023 21:22
Operator : CG/JU
Sample : 02020-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	31.0	ng	2508970	1	7.963	1618110	20.0
(1S)-2,6,6-Trim...	6.640	2.8	ng	229016	1	7.963	1618110	20.0
Juglone	14.851	5.8	ng	733997	3	14.604	2516830	20.0
Benzophenone	15.963	3.1	ng	391573	3	14.604	2516830	20.0
n-Hexadecanoic ...	18.245	12.7	ng	1752750	4	17.351	2762650	20.0
Octadecanoic acid	19.515	3.4	ng	633994	5	21.527	3759900	20.0
3-Phenylpropyl ...	20.562	4.1	ng	766161	5	21.527	3759900	20.0
2-Bromo-2',5'-d...	20.815	10.9	ng	2048530	5	21.527	3759900	20.0
Cinnamyl cinnamate	21.074	13.9	ng	2611020	5	21.527	3759900	20.0
1-Tetracosene	21.233	5.6	ng	1055180	5	21.527	3759900	20.0
2-Methyl-2-doco...	22.168	4.4	ng	823172	5	21.527	3759900	20.0
Docosane, 11-bu...	24.574	14.7	ng	2389840	6	23.956	3243720	20.0