

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032823\
 Data File : BM039185.D
 Acq On : 28 Mar 2023 18:32
 Operator : CG/JU
 Sample : 02111-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 APCS-SOUTH

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: BM039185.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	289	296	304	rBV	1989700	2717670	27.91%	3.922%
2	5.493	369	375	388	rBV	4414278	6446838	66.22%	9.304%
3	7.104	641	649	665	rVB	4440664	6830293	70.16%	9.858%
4	7.934	783	790	798	rBV	1125340	1747737	17.95%	2.522%
5	9.104	981	989	1000	rBV	2586979	4182331	42.96%	6.036%
6	10.745	1260	1268	1279	rBV	1412272	2401390	24.67%	3.466%
7	13.204	1679	1686	1698	rBV	6045565	8618083	88.52%	12.438%
8	14.580	1913	1920	1929	rBV	2120003	3032905	31.15%	4.377%
9	15.939	2145	2151	2161	rVB	1535492	2061069	21.17%	2.975%
10	16.068	2166	2173	2188	rVV	4525495	6391674	65.65%	9.225%
11	16.498	2241	2246	2253	rVB	200194	265749	2.73%	0.384%
12	16.645	2264	2271	2276	rBV	103524	154558	1.59%	0.223%
13	16.721	2276	2284	2292	rBV2	74946	128558	1.32%	0.186%
14	17.327	2381	2387	2395	rVB	2294826	3291328	33.81%	4.750%
15	18.092	2513	2517	2528	rBV4	65633	117806	1.21%	0.170%
16	18.221	2534	2539	2550	rBV	1355301	2110518	21.68%	3.046%
17	19.374	2732	2735	2744	rVB3	68114	122294	1.26%	0.176%
18	19.497	2751	2756	2773	rBV	366954	727379	7.47%	1.050%
19	19.945	2827	2832	2841	rBV	7714679	9735957	100.00%	14.051%
20	20.250	2882	2884	2888	rVB	110273	111324	1.14%	0.161%
21	20.750	2966	2969	2972	rVB	109589	109441	1.12%	0.158%
22	21.209	3044	3047	3056	rBV	637756	849477	8.73%	1.226%
23	21.509	3093	3098	3104	rBV	2347642	3131991	32.17%	4.520%
24	22.756	3307	3310	3317	rVB	669047	964781	9.91%	1.392%
25	23.927	3503	3509	3520	rVB2	1499872	3038754	31.21%	4.386%

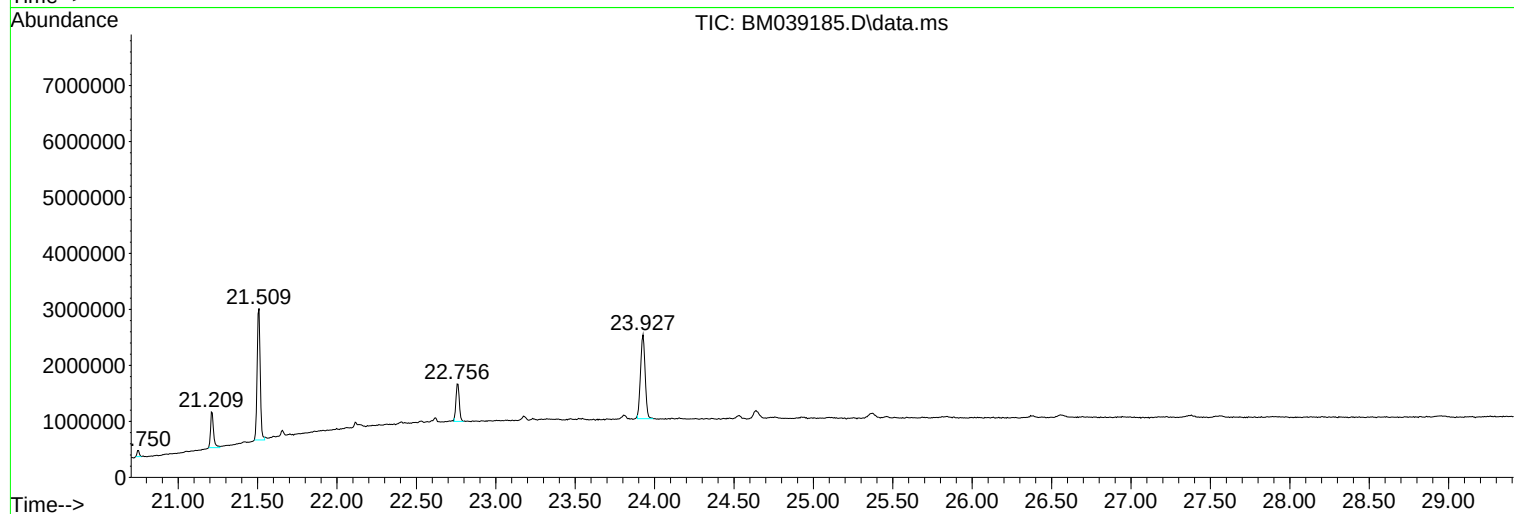
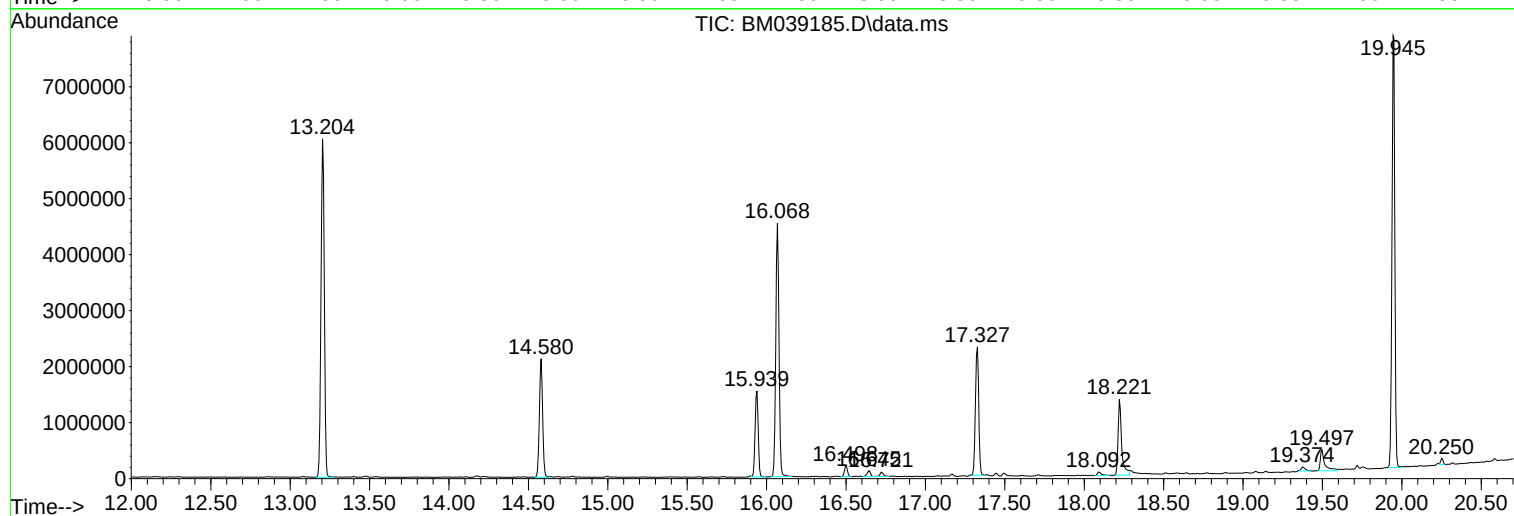
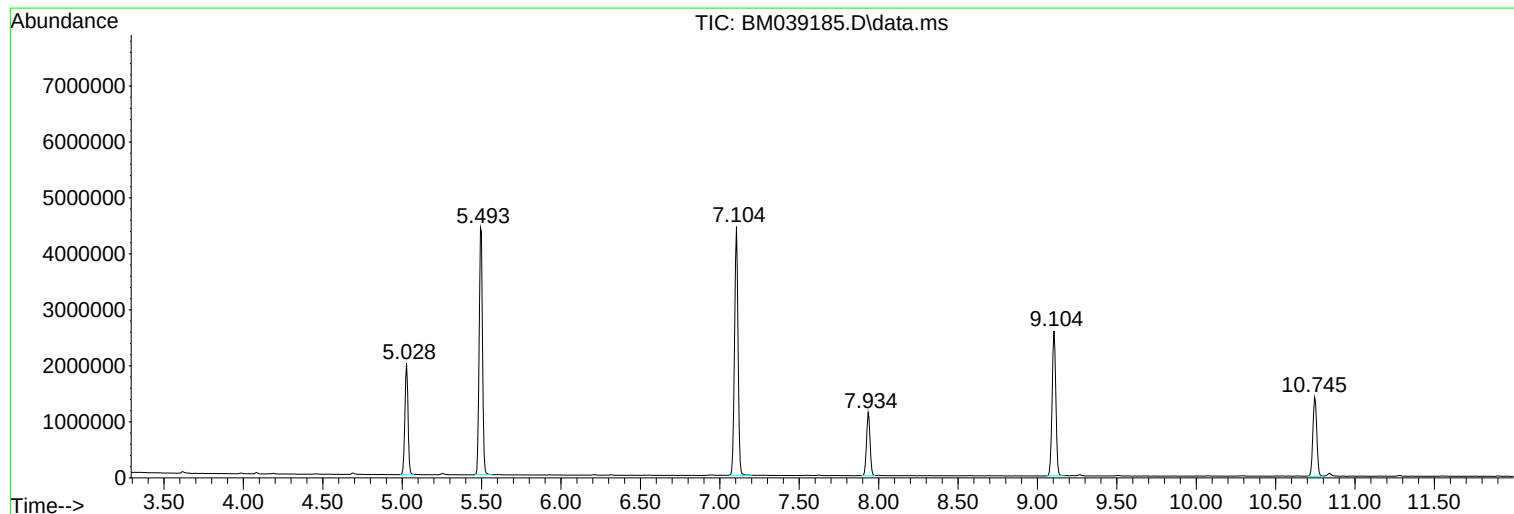
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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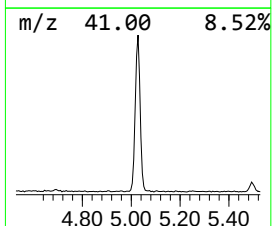
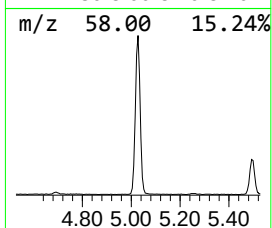
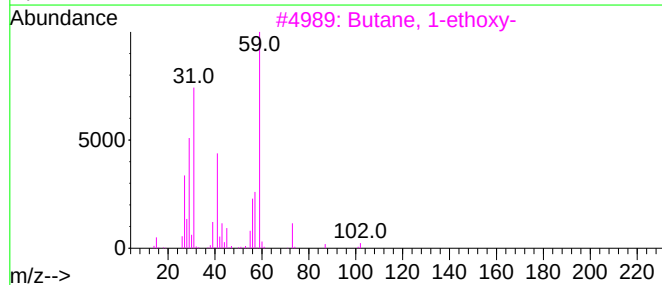
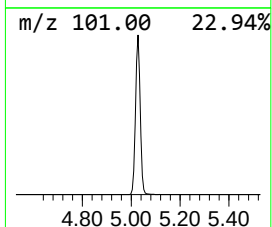
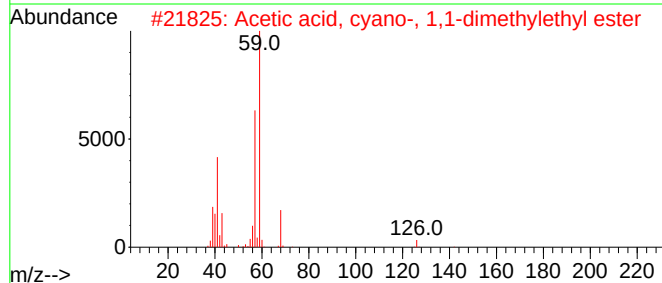
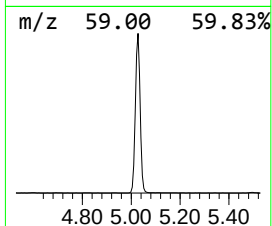
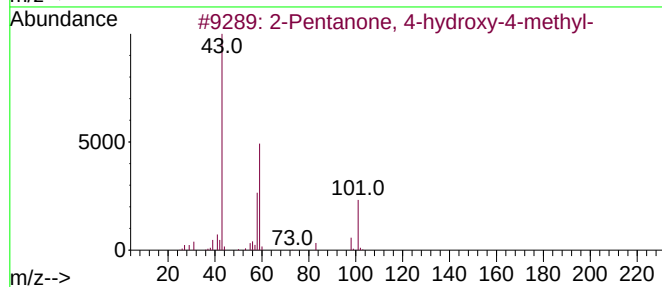
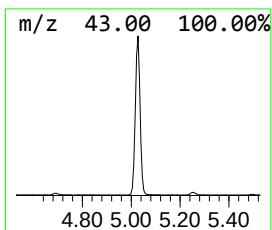
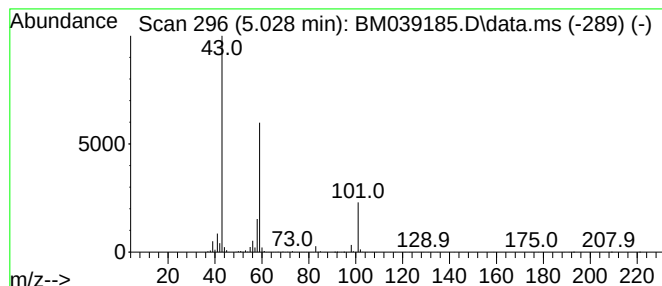
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.028	31.10 ng	2717670	1,4-Dichlorobenzene-d4	7.934

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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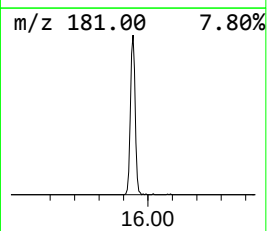
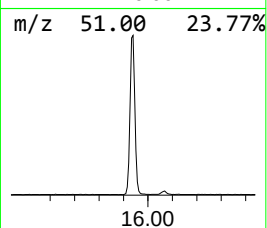
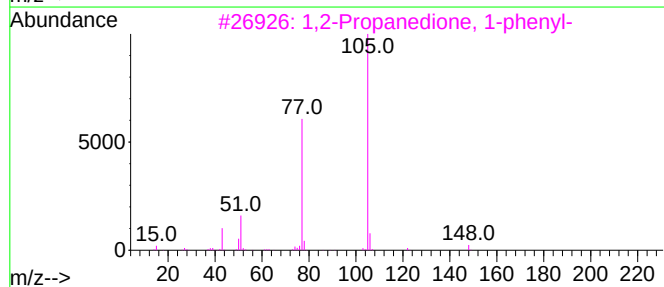
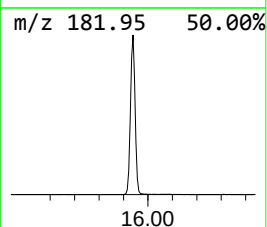
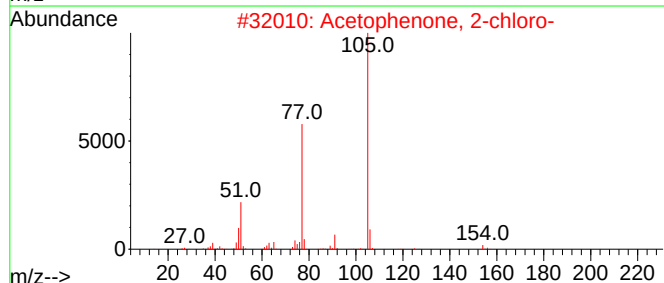
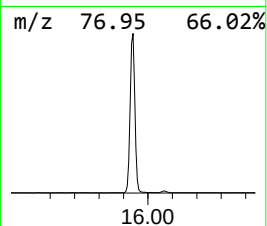
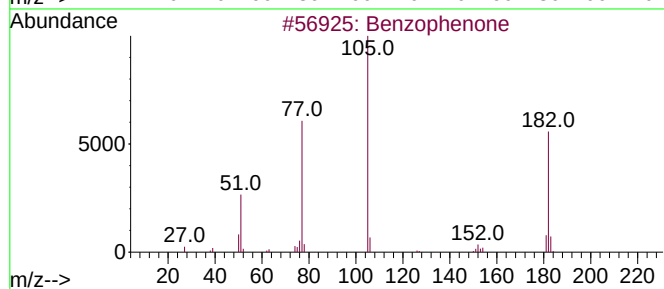
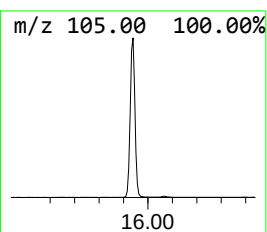
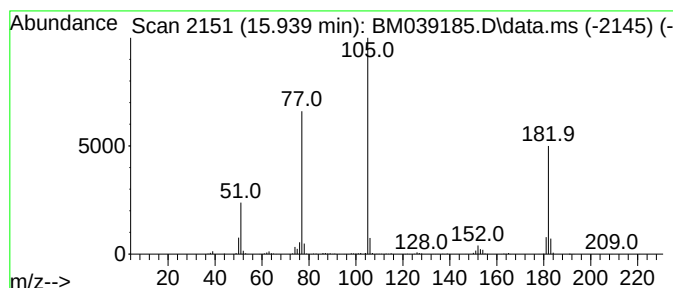
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.939	13.59 ng	2061070	Acenaphthene-d10	14.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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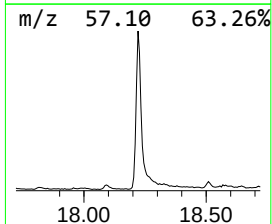
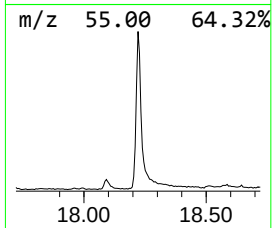
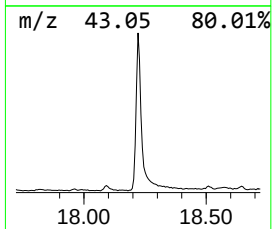
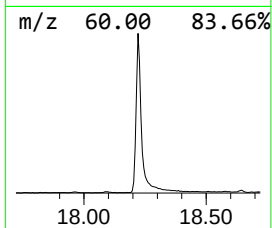
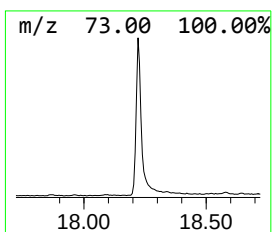
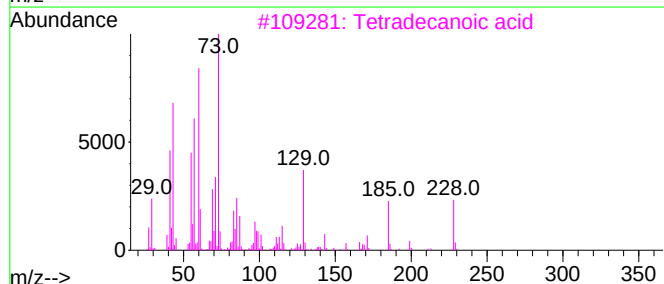
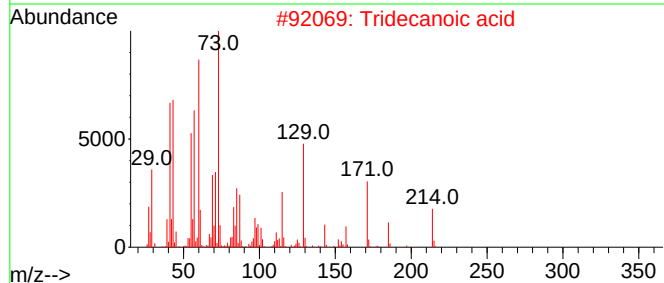
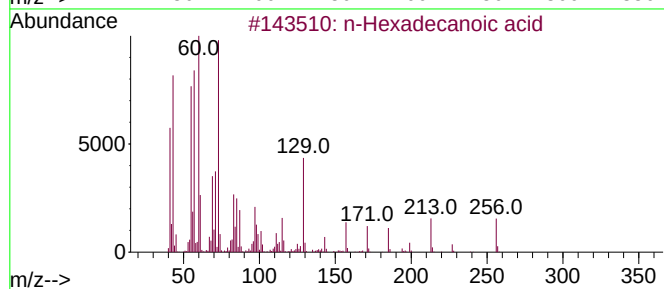
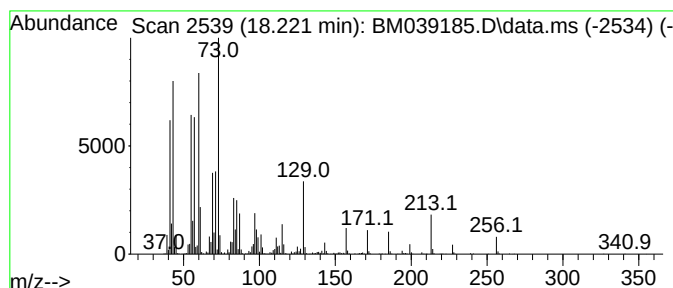
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.221	12.82 ng	2110520	Phenanthrene-d10		17.327	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	55



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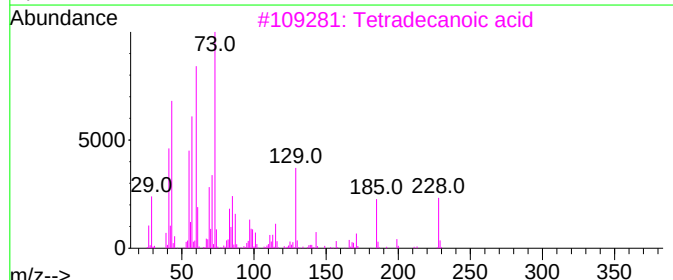
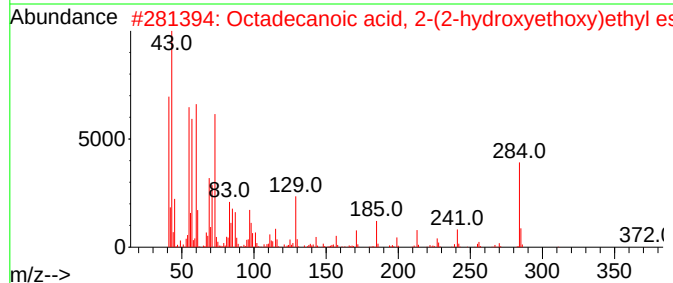
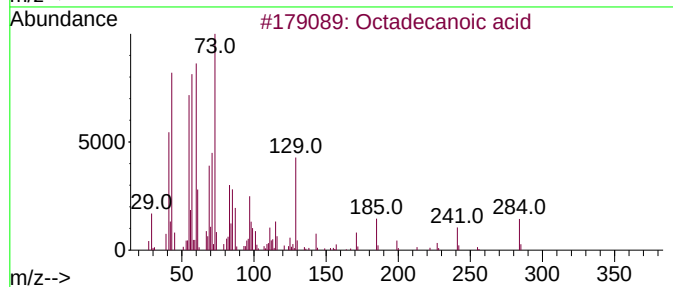
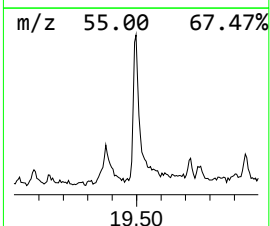
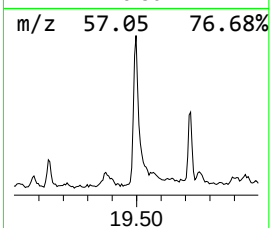
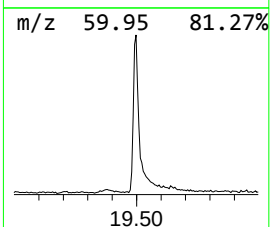
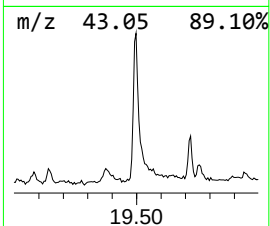
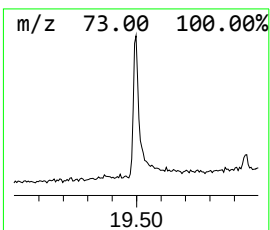
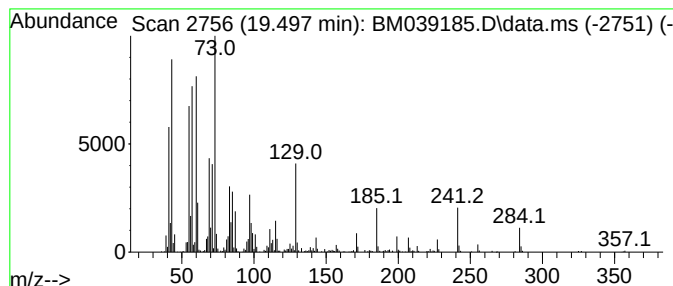
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.497	4.64 ng	727379	Chrysene-d12	21.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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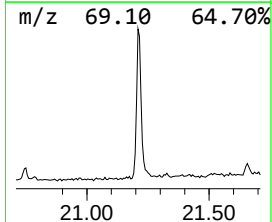
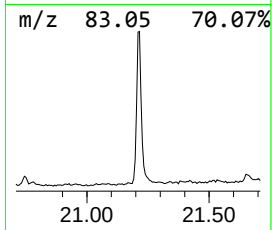
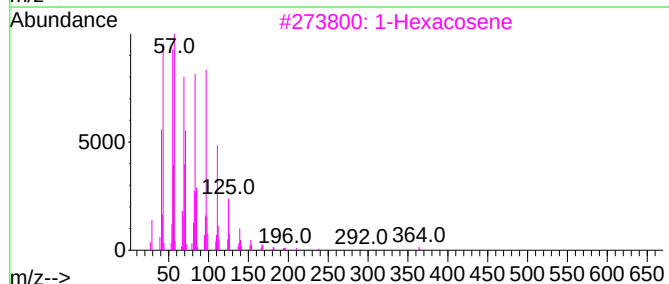
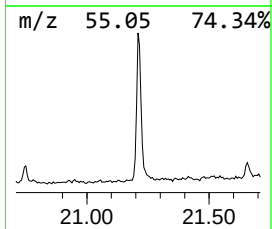
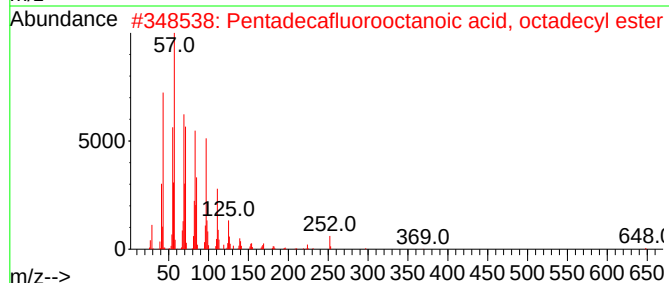
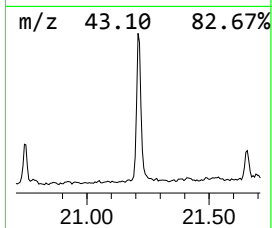
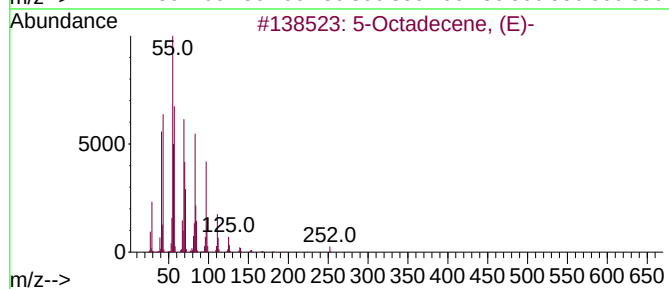
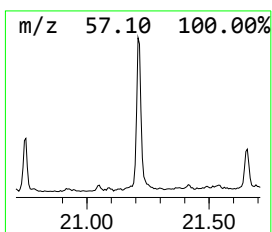
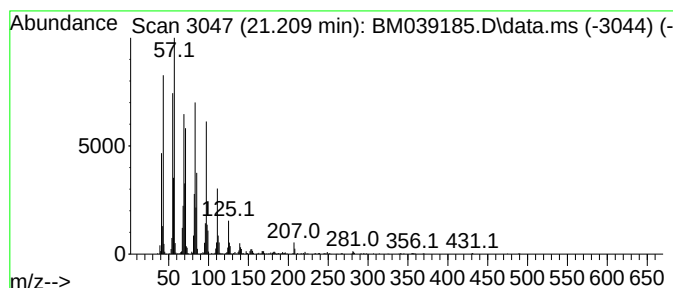
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Peak Number 5 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.209	5.42 ng	849477	Chrysene-d12	21.509	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



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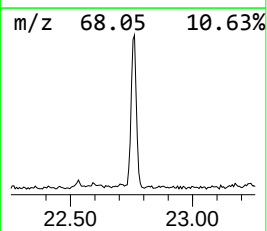
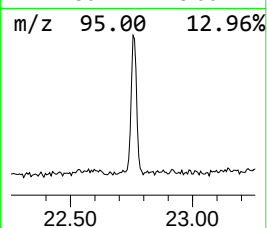
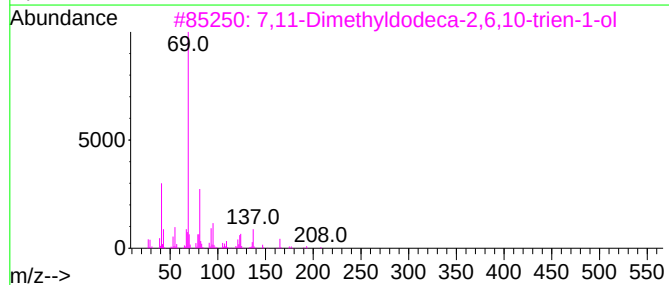
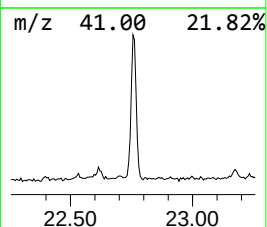
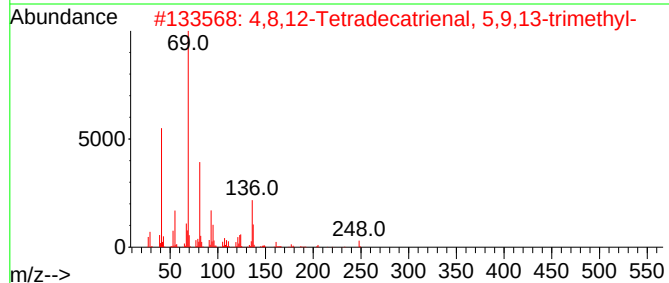
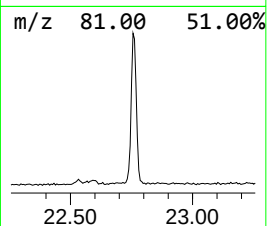
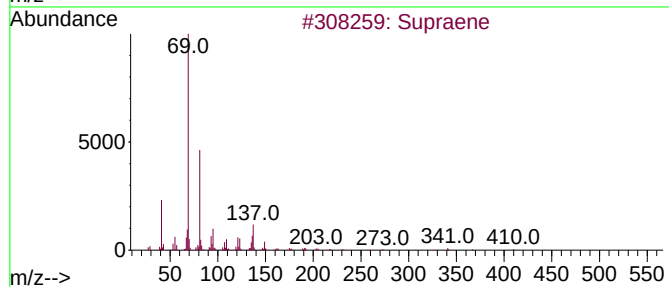
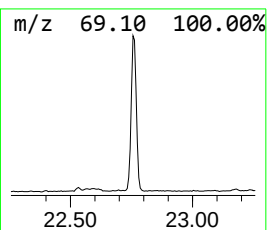
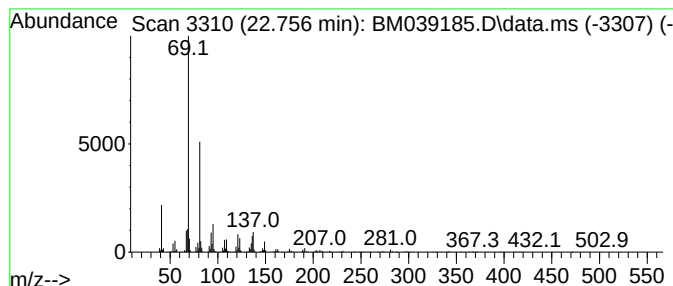
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.756	6.35 ng	964781	Perylene-d12	23.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032823\
Data File : BM039185.D
Acq On : 28 Mar 2023 18:32
Operator : CG/JU
Sample : 02111-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
APCS-SOUTH

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-...	5.028	31.1	ng	2717670	1	7.934	1747740	20.0
Benzophenone	15.939	13.6	ng	2061070	3	14.580	3032910	20.0
n-Hexadecanoic ...	18.221	12.8	ng	2110520	4	17.327	3291330	20.0
Octadecanoic acid	19.497	4.6	ng	727379	5	21.509	3131990	20.0
5-Octadecene, (E)-	21.209	5.4	ng	849477	5	21.509	3131990	20.0
Supraene	22.756	6.3	ng	964781	6	23.927	3038750	20.0