

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
 Data File : BM039163.D
 Acq On : 27 Mar 2023 16:47
 Operator : CG/JU
 Sample : 02090-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DS-01-032323

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: BM039163.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	290	297	304	rBV	578317	829778	5.54%	1.337%
2	5.498	370	376	388	rBV	980365	1387018	9.26%	2.235%
3	7.104	639	649	660	rBV	544091	852506	5.69%	1.374%
4	7.939	785	791	798	rBV	923298	1426434	9.52%	2.298%
5	9.110	983	990	1006	rBV	2944742	4850789	32.38%	7.816%
6	10.751	1260	1269	1277	rBV	1183530	1956072	13.06%	3.152%
7	13.210	1680	1687	1698	rBV	7280646	10459011	69.82%	16.852%
8	14.586	1914	1921	1930	rVB	1686871	2468087	16.48%	3.977%
9	15.427	2055	2064	2069	rVB2	129355	174164	1.16%	0.281%
10	15.939	2145	2151	2156	rBV	144178	213877	1.43%	0.345%
11	16.074	2166	2174	2181	rBV	3087663	4371351	29.18%	7.043%
12	16.286	2206	2210	2213	rBV	236543	321342	2.15%	0.518%
13	17.080	2341	2345	2350	rBV	248774	308427	2.06%	0.497%
14	17.327	2382	2387	2394	rBV	2002747	2904032	19.39%	4.679%
15	17.821	2467	2471	2476	rBV	238354	283051	1.89%	0.456%
16	17.998	2497	2501	2506	rVB	159462	193153	1.29%	0.311%
17	18.227	2534	2540	2549	rBV	1699852	2614359	17.45%	4.212%
18	18.515	2585	2589	2593	rBV	217500	261722	1.75%	0.422%
19	19.150	2693	2697	2698	rBV	156310	185962	1.24%	0.300%
20	19.168	2698	2700	2704	rVB	174085	178188	1.19%	0.287%
21	19.497	2752	2756	2770	rBV	839940	1443117	9.63%	2.325%
22	19.727	2791	2795	2797	rBV	129772	166200	1.11%	0.268%
23	19.950	2828	2833	2839	rBV	11779704	14980514	100.00%	24.137%
24	20.256	2882	2885	2889	rVB	145521	158642	1.06%	0.256%
25	21.215	3044	3048	3057	rBV	903652	1190814	7.95%	1.919%
26	21.509	3093	3098	3103	rBV	2738494	3456213	23.07%	5.569%
27	22.768	3309	3312	3320	rVB	453111	621548	4.15%	1.001%
28	23.932	3504	3510	3518	rVB2	1944823	3807641	25.42%	6.135%

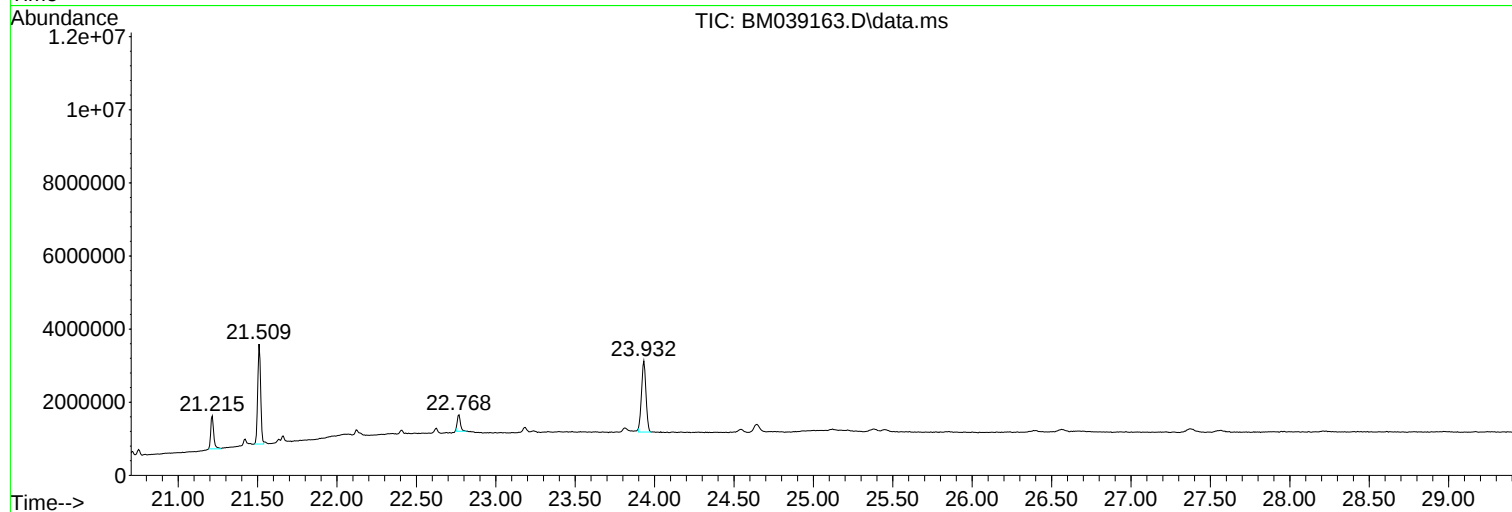
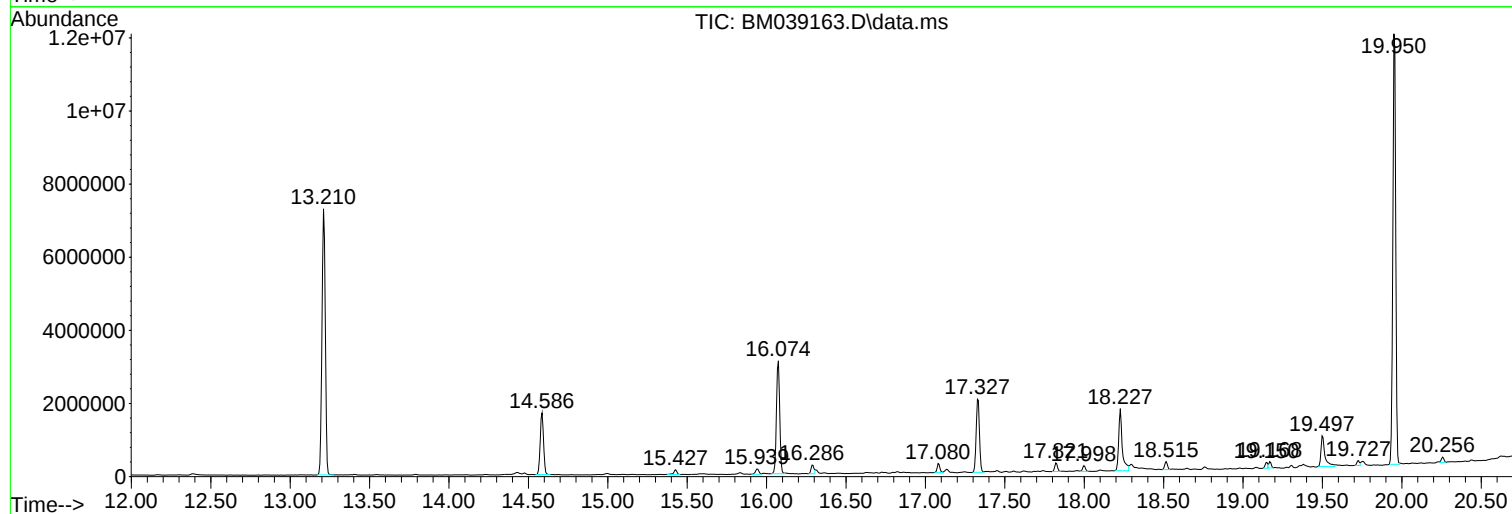
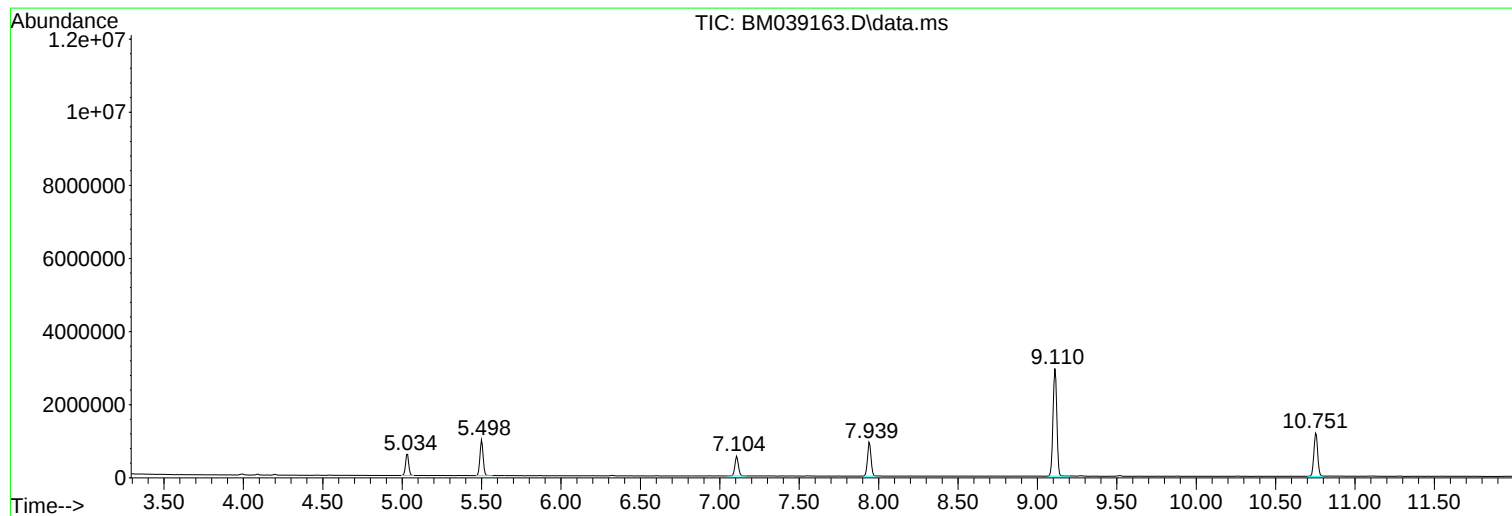
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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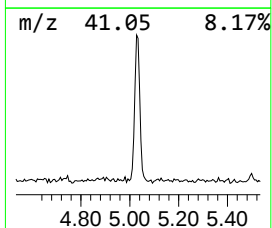
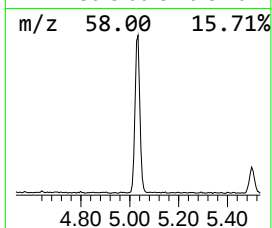
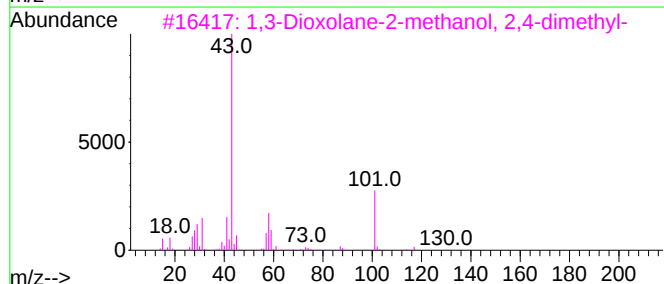
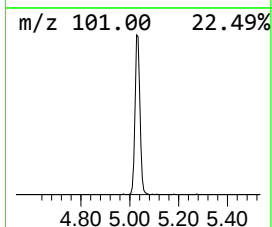
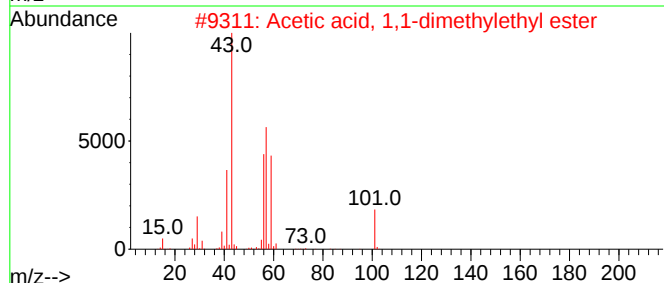
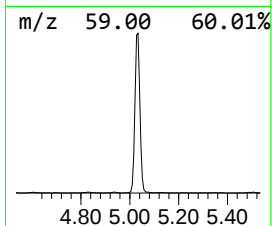
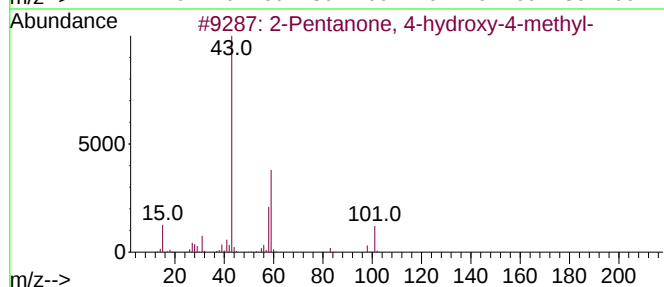
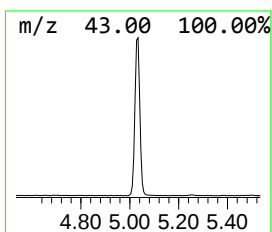
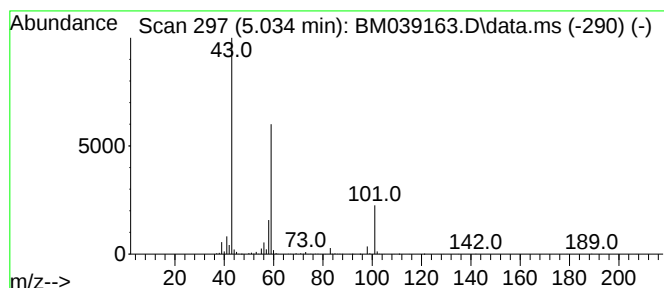
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	11.63 ng	829778	1,4-Dichlorobenzene-d4	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		



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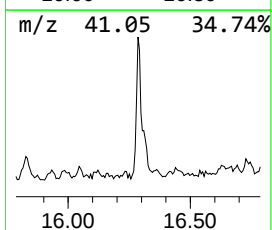
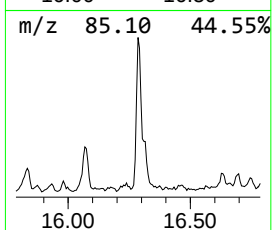
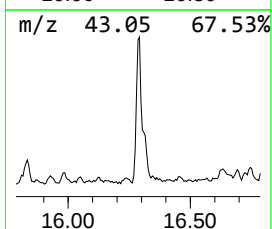
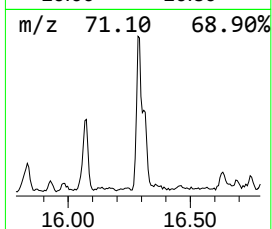
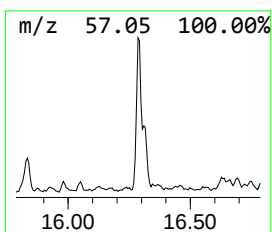
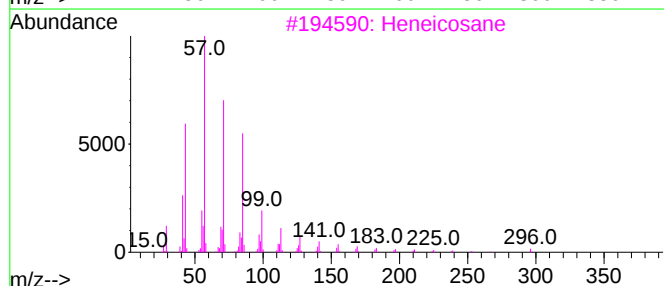
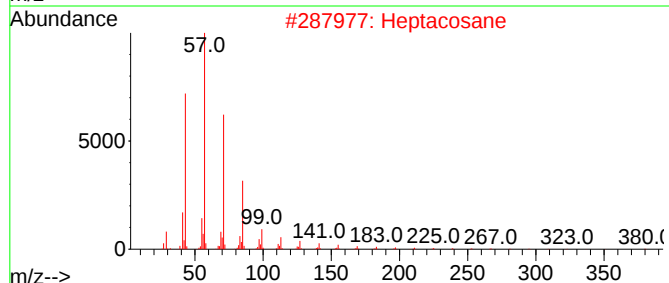
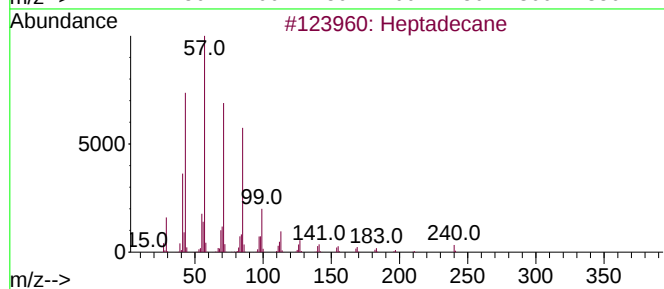
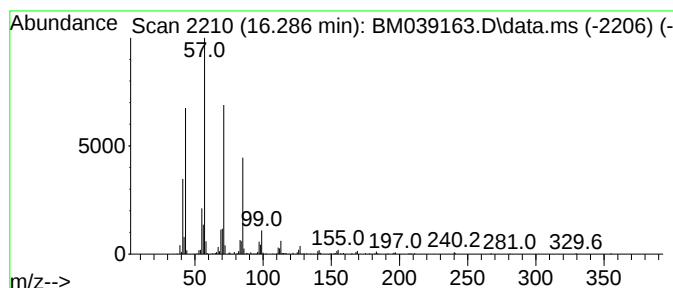
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Peak Number 2 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.286	2.21 ng	321342	Phenanthrene-d10	17.327

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	97
2		Heptacosane	380	C27H56	000593-49-7	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Nonadecane	268	C19H40	000629-92-5	90
5		Decane, 5-propyl-	184	C13H28	017312-62-8	90



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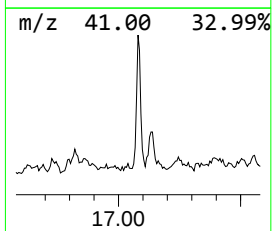
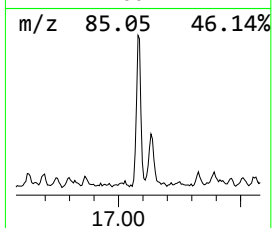
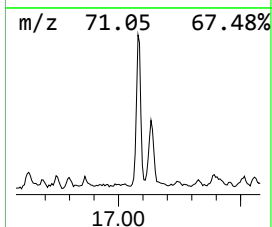
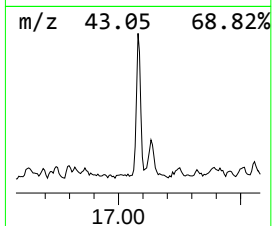
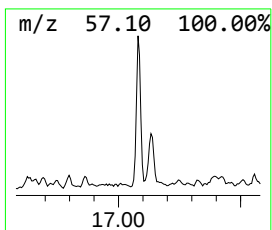
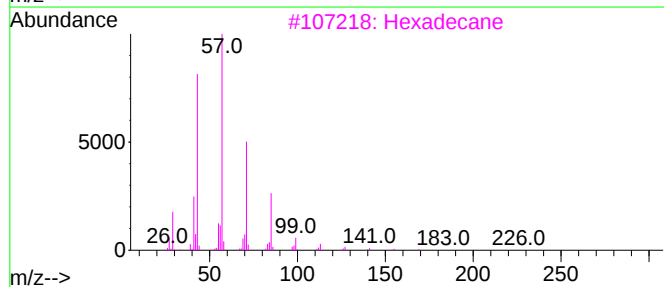
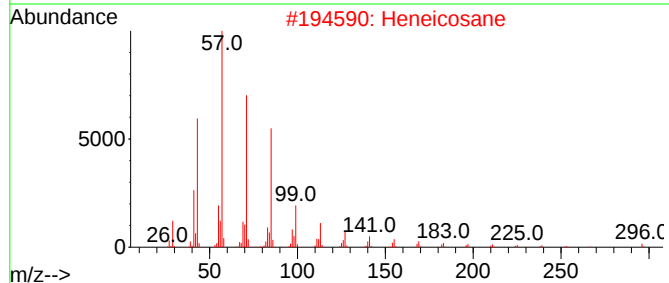
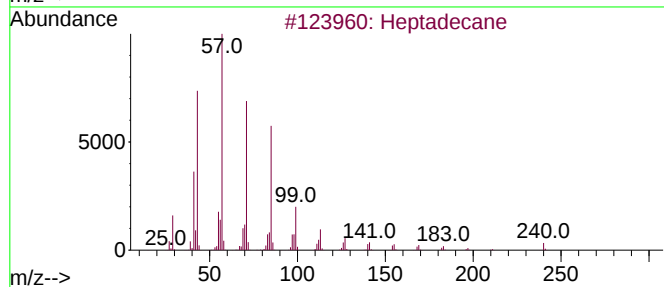
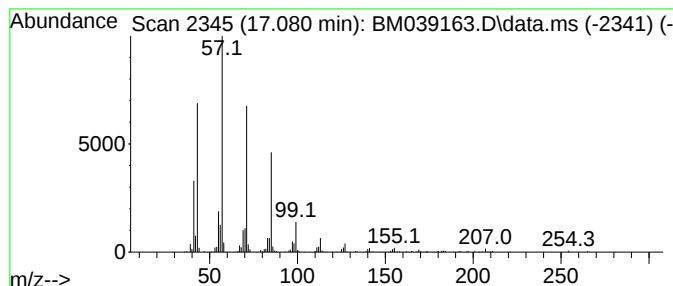
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.080	2.12 ng	308427	Phenanthrene-d10	17.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hexadecane	226	C16H34	000544-76-3	90
4			Pentadecane	212	C15H32	000629-62-9	90
5			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90



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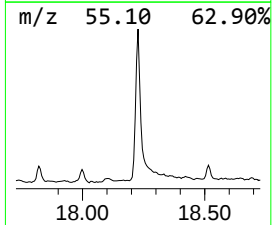
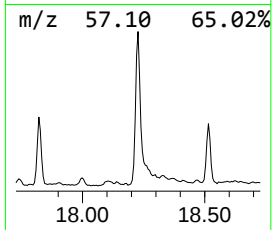
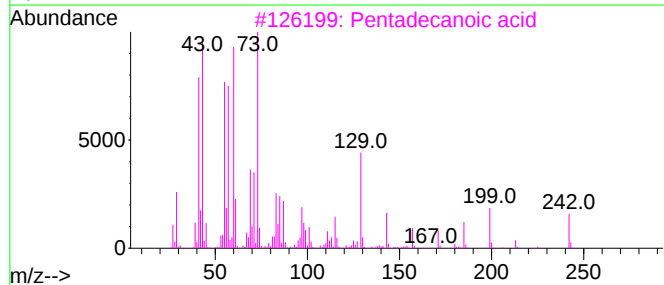
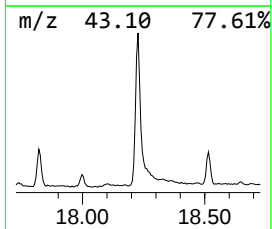
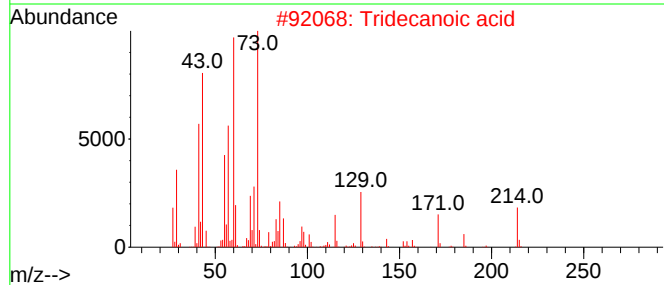
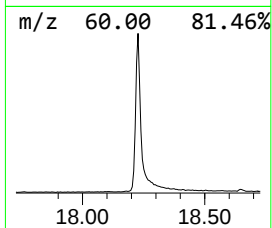
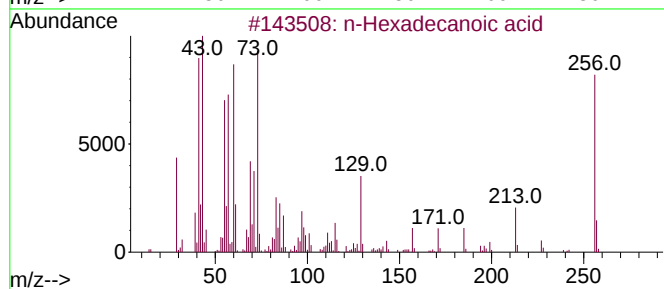
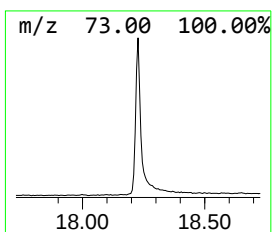
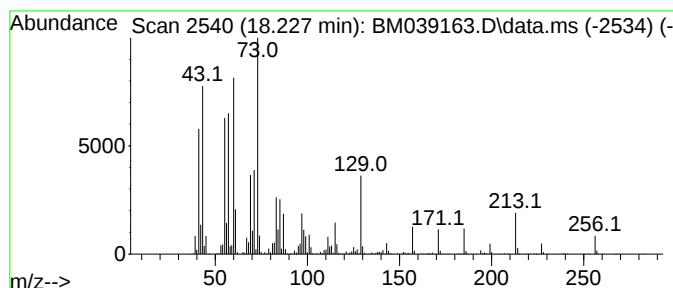
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	18.00 ng	2614360	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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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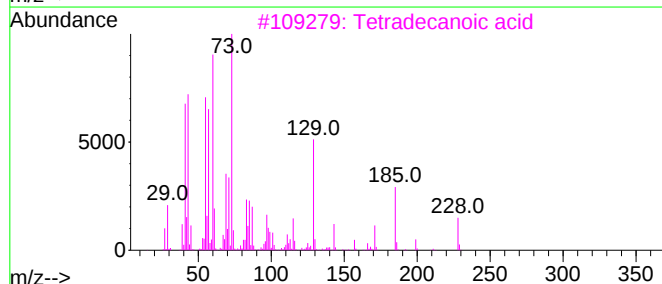
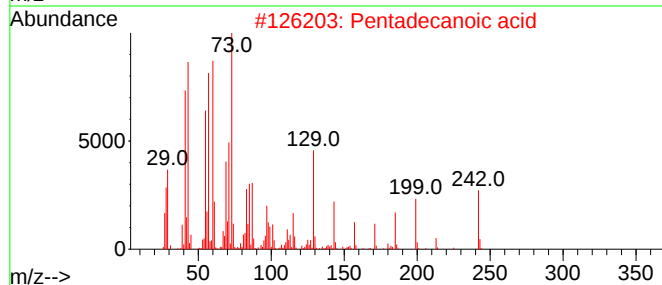
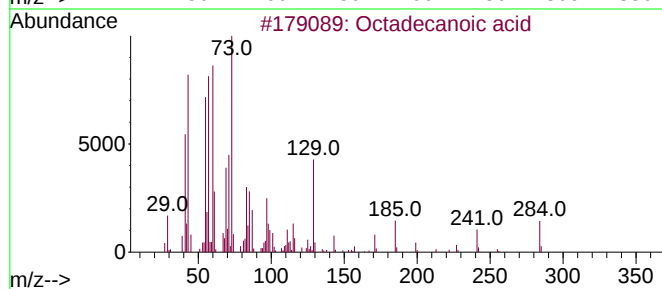
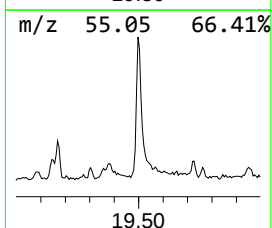
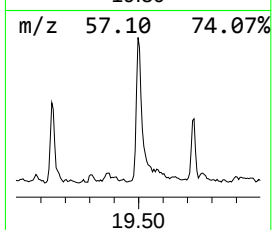
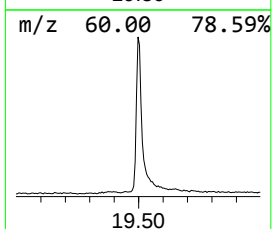
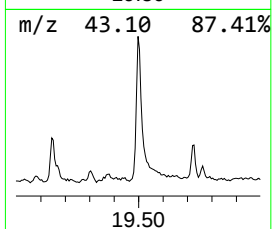
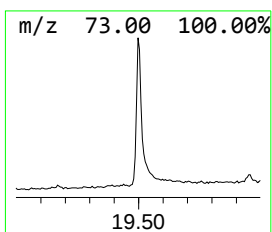
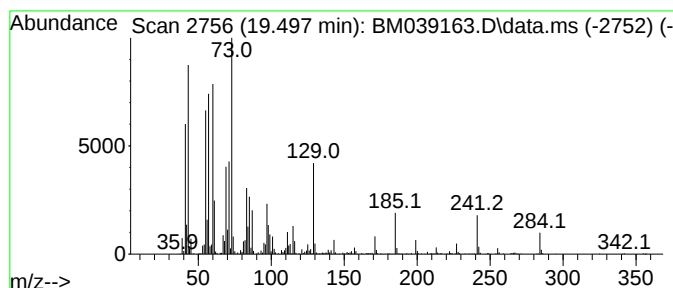
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.497	8.35 ng	1443120	Chrysene-d12	21.509

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	81
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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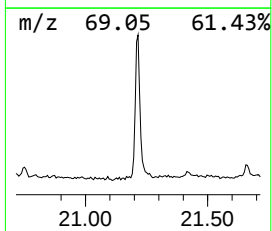
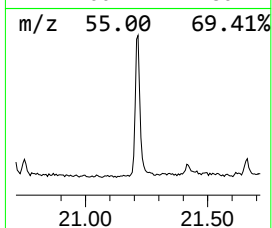
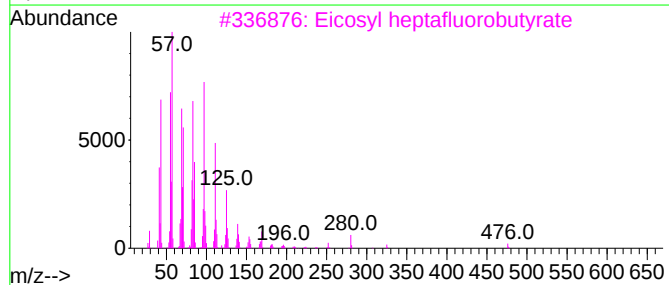
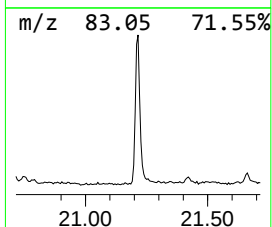
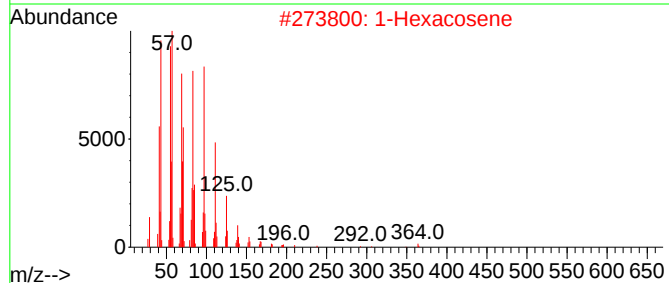
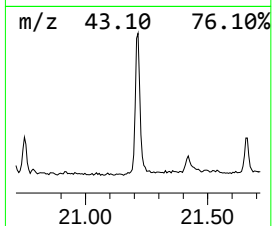
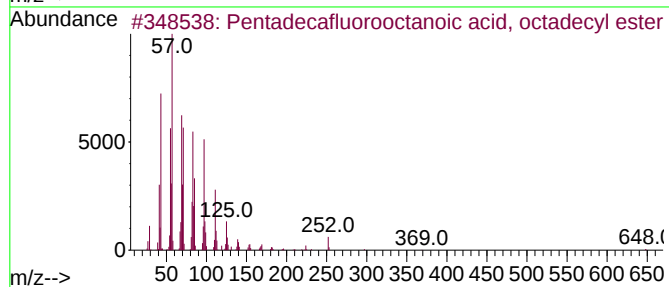
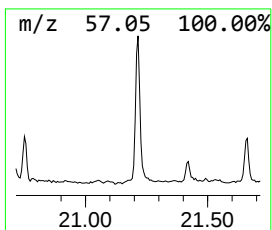
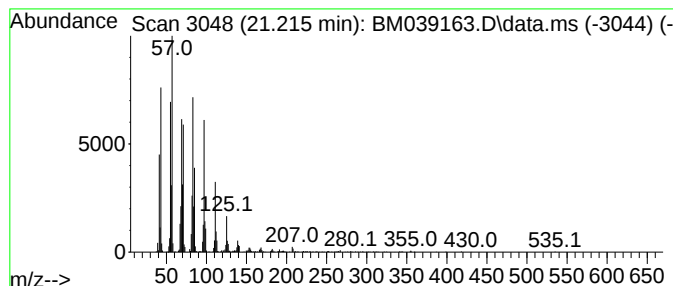
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.215	6.89 ng	1190810	Chrysene-d12	21.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			1-Hexacosene	364	C26H52	018835-33-1	91
3			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039163.D
Acq On : 27 Mar 2023 16:47
Operator : CG/JU
Sample : 02090-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DS-01-032323

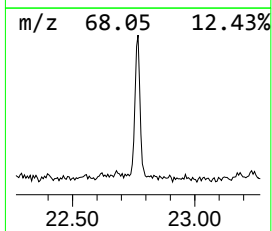
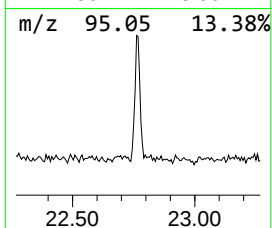
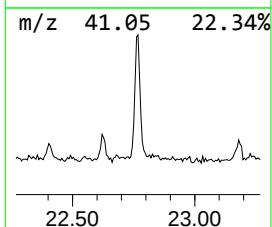
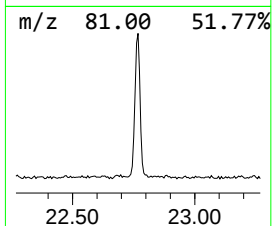
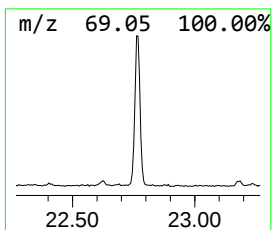
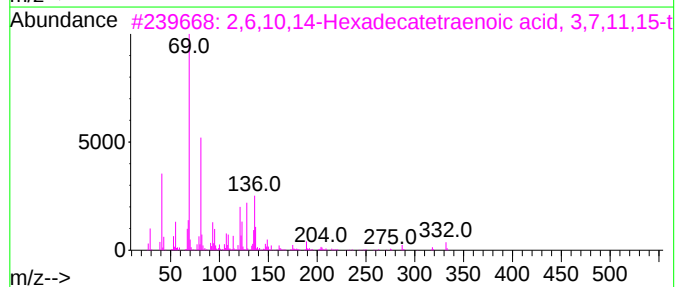
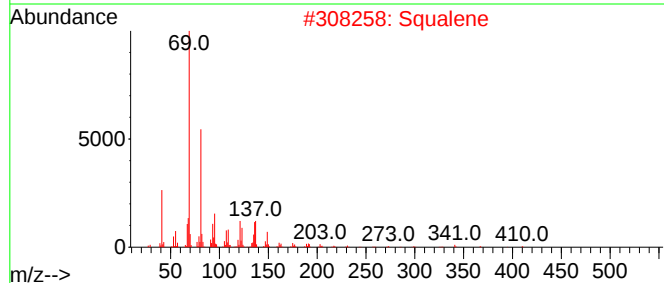
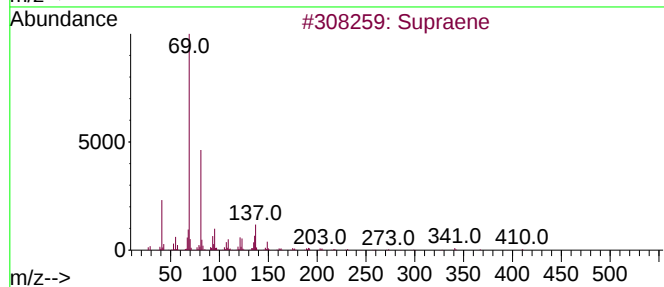
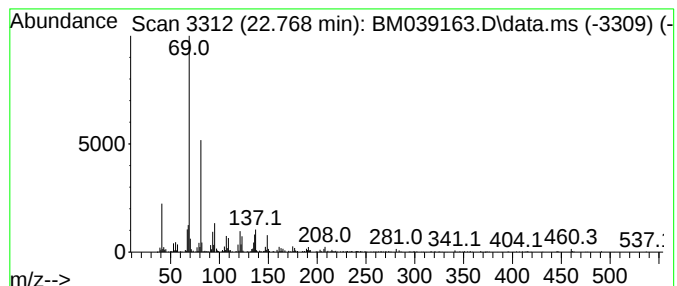
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.768	3.26 ng	621548	Perylene-d12	23.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	93
2			Squalene	410	C30H50	000111-02-4	91
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			trans-Farnesol	222	C15H26O	000106-28-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039163.D
Acq On : 27 Mar 2023 16:47
Operator : CG/JU
Sample : 02090-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DS-01-032323

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-...	5.034	11.6	ng	829778	1	7.939	1426430	20.0
Heptadecane	16.286	2.2	ng	321342	4	17.327	2904030	20.0
Heneicosane	17.080	2.1	ng	308427	4	17.327	2904030	20.0
n-Hexadecanoic ...	18.227	18.0	ng	2614360	4	17.327	2904030	20.0
Octadecanoic acid	19.497	8.3	ng	1443120	5	21.509	3456210	20.0
Pentadecafluoro...	21.215	6.9	ng	1190810	5	21.509	3456210	20.0
Supraene	22.768	3.3	ng	621548	6	23.933	3807640	20.0