

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
 Data File : BG055590.D
 Acq On : 12 Nov 2022 15:11
 Operator : CG/JU
 Sample : N5431-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20221170-COMP-05-MODIFIED-ELUTRIATE

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_G\Methods\8270-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.324	3	6	26	rVB	587997	894539	42.82%	6.371%
2	4.710	235	242	247	rBV	14598	23989	1.15%	0.171%
3	5.321	341	346	354	rVB	47213	74920	3.59%	0.534%
4	5.791	419	426	433	rBV	232088	376112	18.00%	2.679%
5	7.401	691	700	709	rBV	194317	342166	16.38%	2.437%
6	8.271	840	848	860	rBV	234838	407314	19.50%	2.901%
7	9.440	1039	1047	1054	rBV	268277	476813	22.82%	3.396%
8	11.097	1321	1329	1337	rBV	323195	582569	27.88%	4.149%
9	13.512	1731	1740	1749	rVB	760509	1175317	56.25%	8.370%
10	14.887	1967	1974	1984	rVB	569175	901595	43.15%	6.421%
11	16.367	2219	2226	2233	rBV	735397	1113960	53.32%	7.934%
12	16.555	2253	2258	2262	rBV4	12400	22669	1.09%	0.161%
13	16.996	2328	2333	2337	rBV2	23462	32747	1.57%	0.233%
14	17.630	2433	2441	2448	rBV	795002	1247171	59.69%	8.882%
15	17.766	2460	2464	2469	rVB3	14661	20995	1.00%	0.150%
16	18.271	2546	2550	2556	rVB2	39821	51136	2.45%	0.364%
17	18.365	2561	2566	2573	rVV4	15347	25957	1.24%	0.185%
18	18.488	2582	2587	2596	rBV	297569	446634	21.38%	3.181%
19	19.428	2744	2747	2752	rVB3	20255	25165	1.20%	0.179%
20	19.628	2778	2781	2790	rVB8	22424	44584	2.13%	0.318%
21	19.746	2797	2801	2814	rBV	118333	193913	9.28%	1.381%
22	20.022	2845	2848	2854	rVB3	22459	33150	1.59%	0.236%
23	20.216	2875	2881	2887	rVB	1541234	2089292	100.00%	14.880%
24	21.532	3100	3105	3118	rBV2	135012	316632	15.15%	2.255%
25	21.925	3165	3172	3179	rBV2	809430	1403316	67.17%	9.994%
26	23.706	3470	3475	3485	rVB2	79342	168520	8.07%	1.200%
27	25.357	3745	3756	3771	rVB2	489803	1550042	74.19%	11.039%

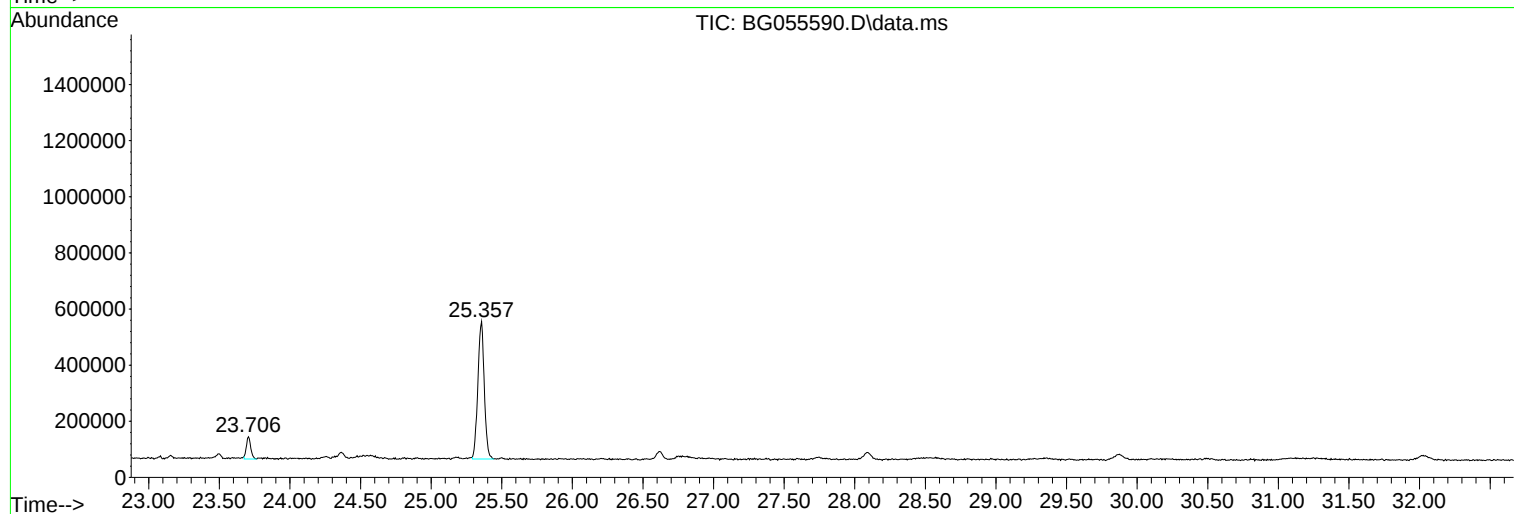
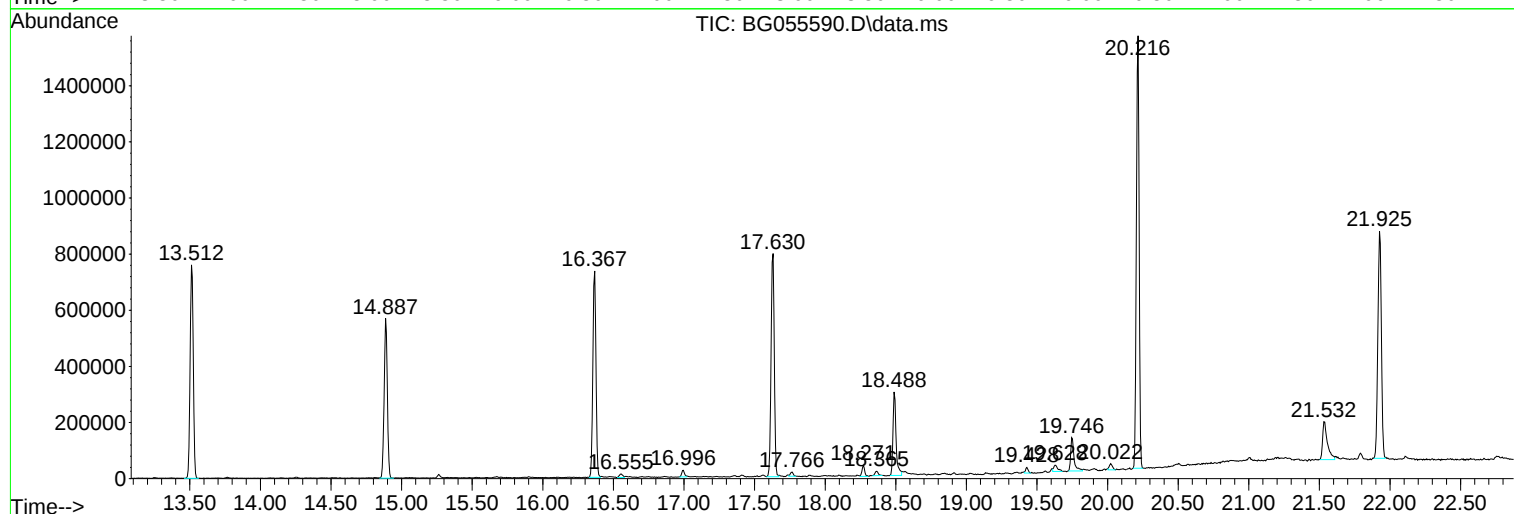
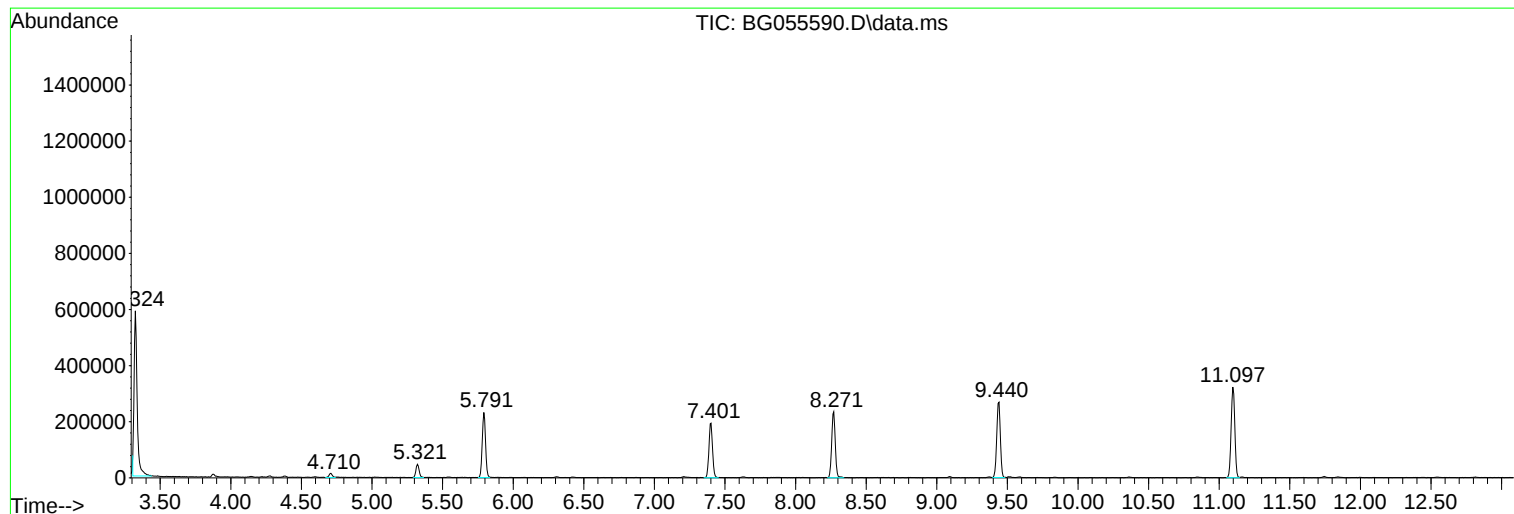
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ClientSampleId :
20221170-COMP-05-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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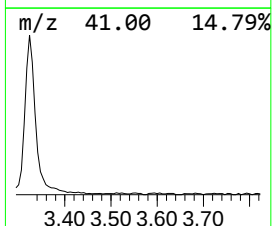
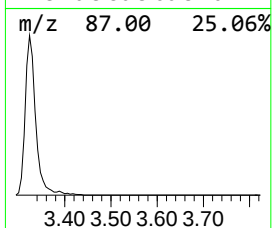
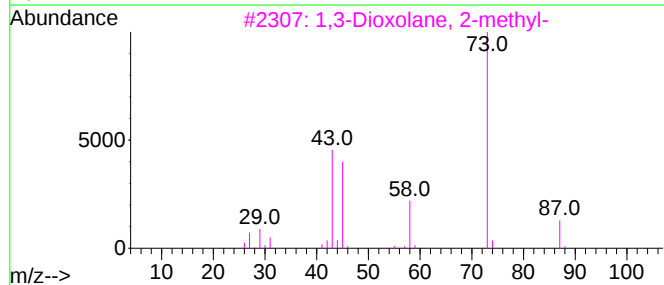
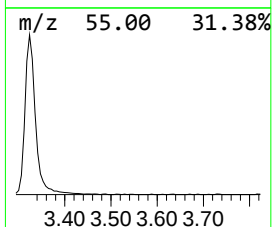
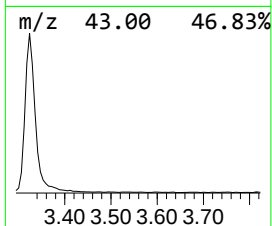
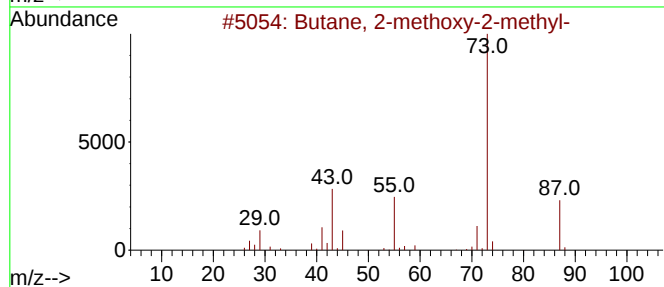
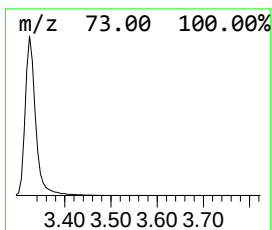
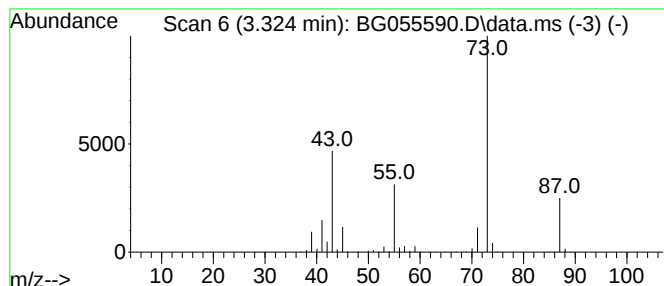
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.324	43.92 ng	894539	1,4-Dichlorobenzene-d4	8.271

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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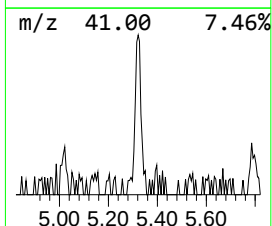
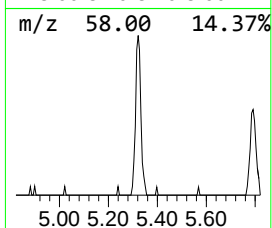
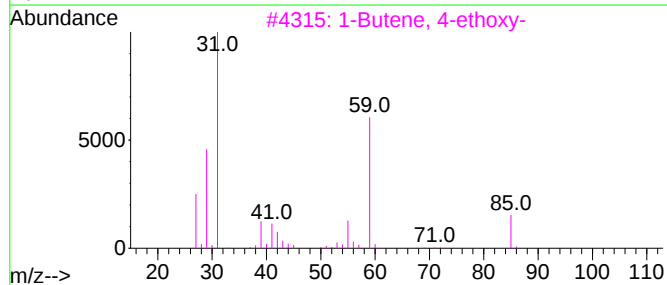
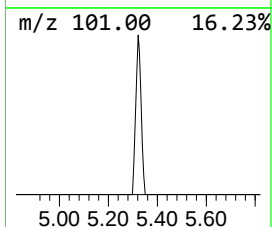
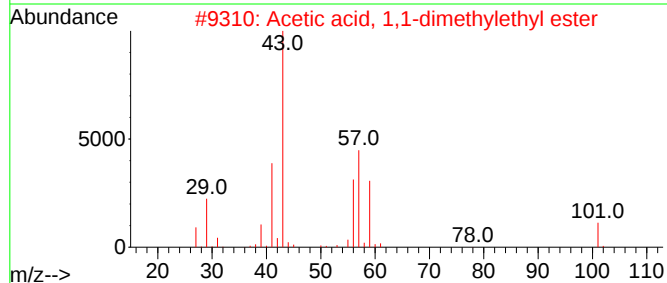
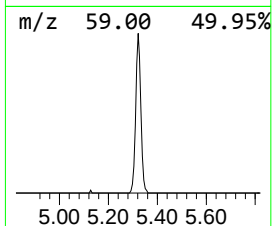
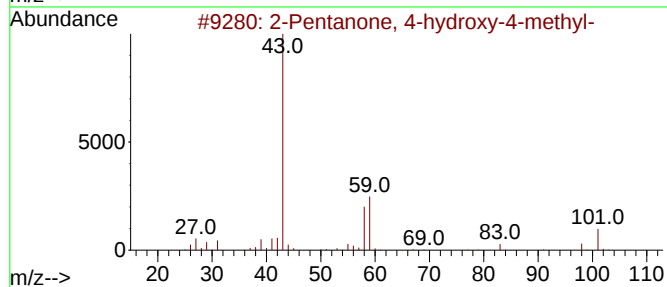
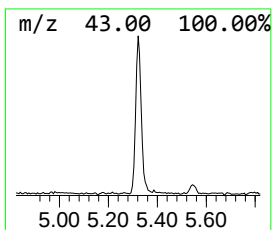
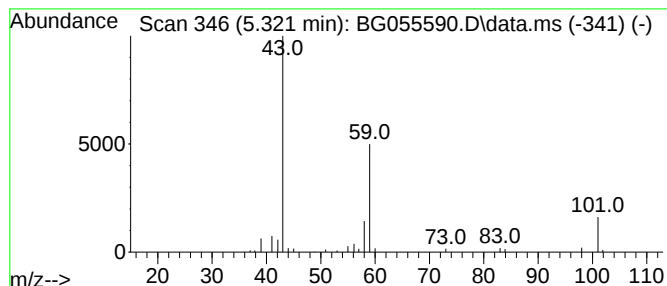
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.321	3.68 ng	74920	1,4-Dichlorobenzene-d4	8.271

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	25		
3	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	17		
4	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		



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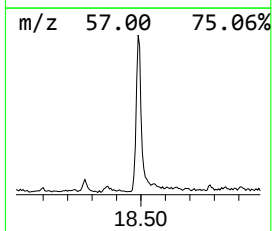
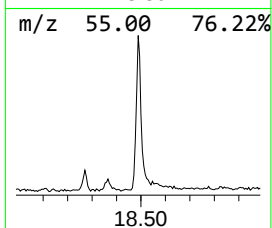
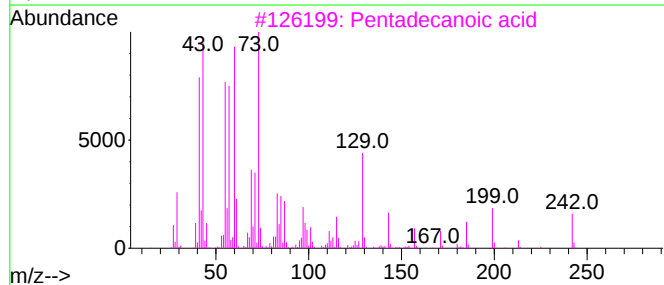
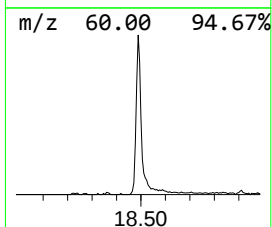
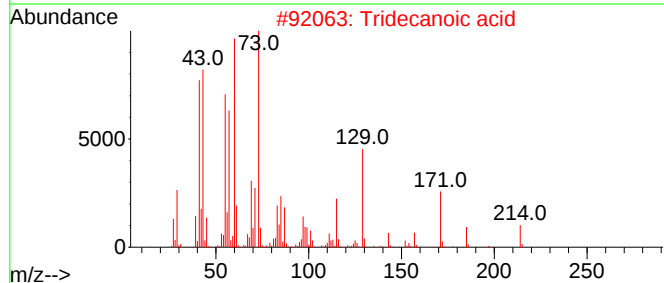
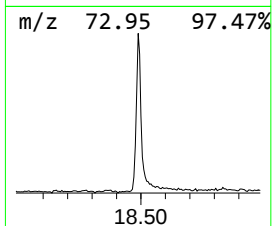
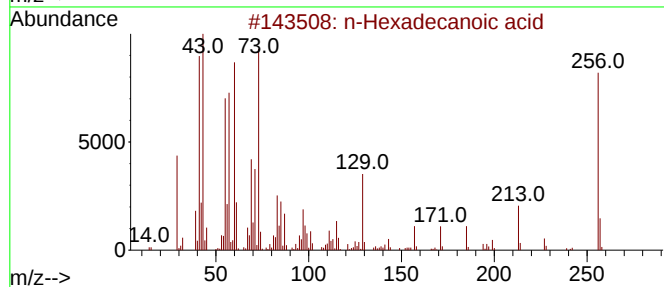
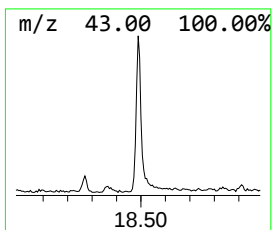
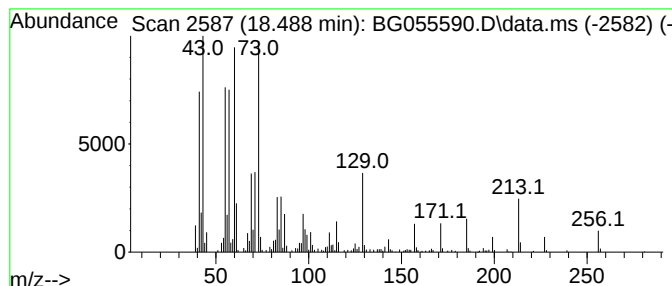
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	7.16 ng	446634	Phenanthrene-d10	17.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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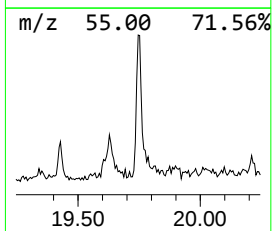
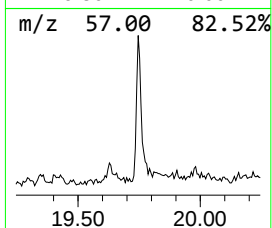
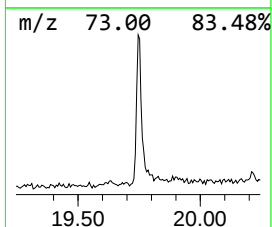
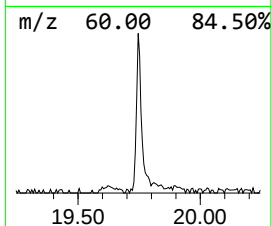
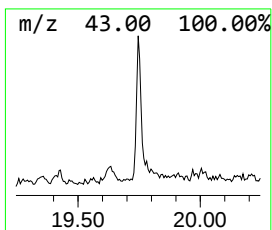
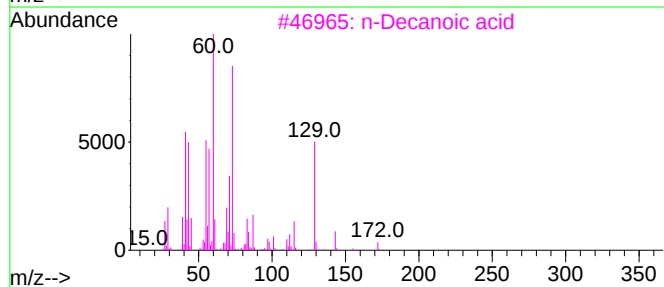
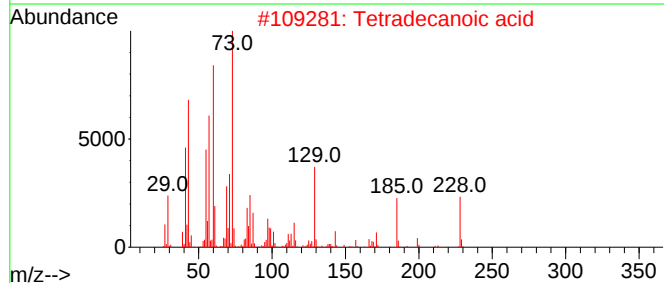
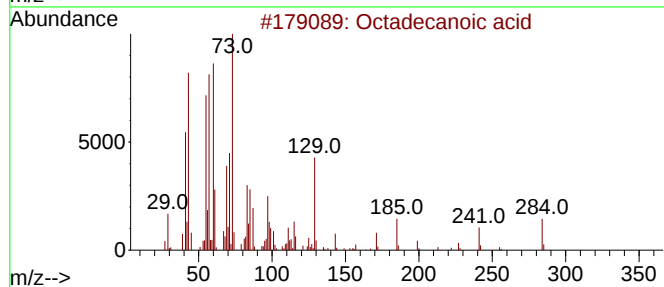
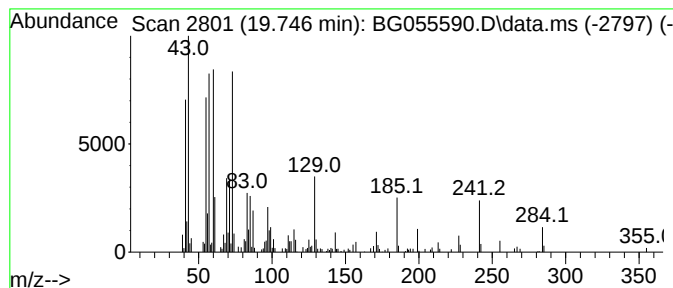
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.746	3.11 ng	193913	Phenanthrene-d10	17.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3			n-Decanoic acid	172	C10H20O2	000334-48-5	70
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	62



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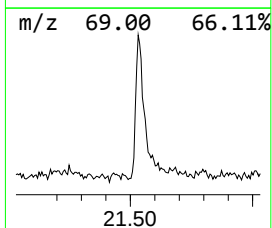
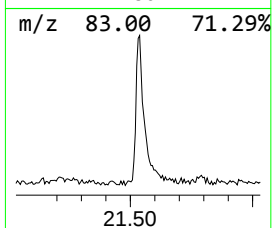
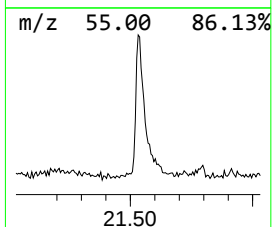
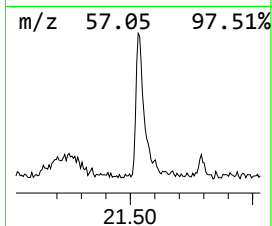
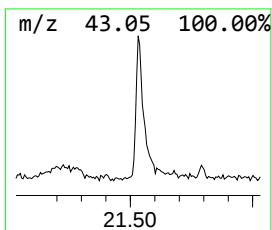
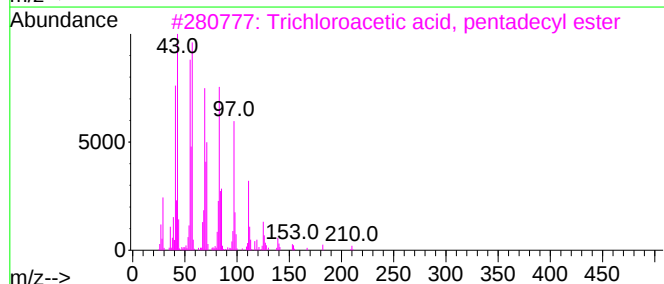
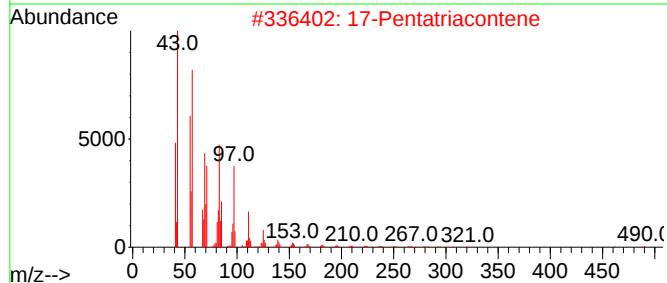
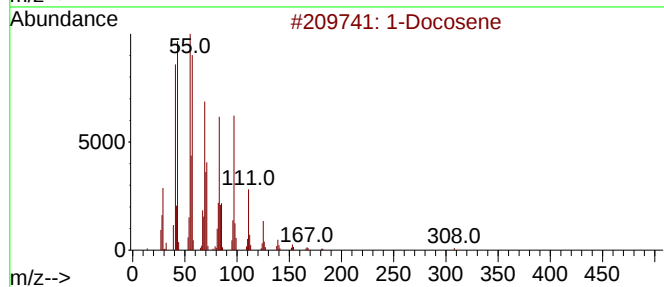
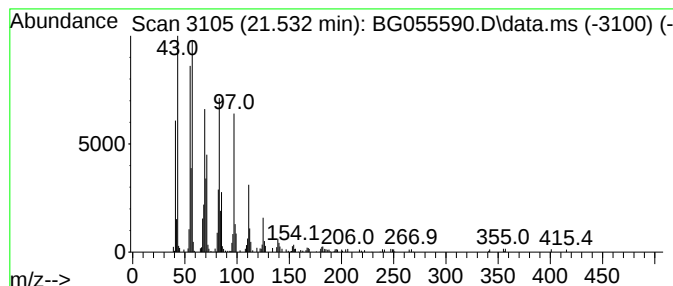
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Peak Number 5 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.532	4.51 ng	316632	Chrysene-d12	21.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	91
2			17-Pentatriacontene	491	C35H70	006971-40-0	91
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4			Octacosanol	410	C28H58O	000557-61-9	91
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



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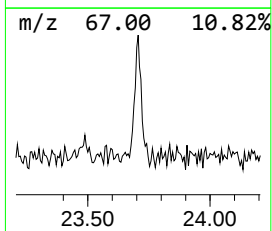
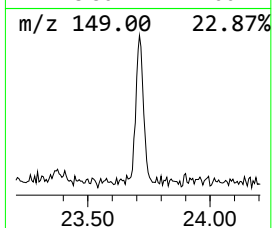
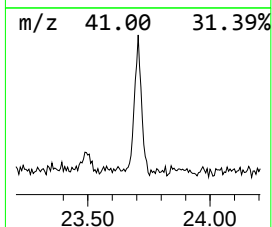
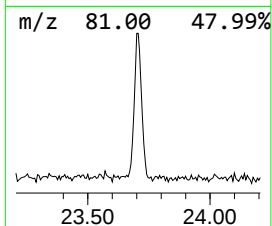
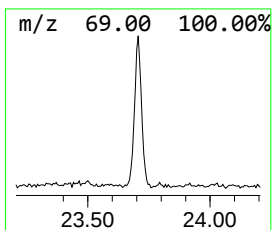
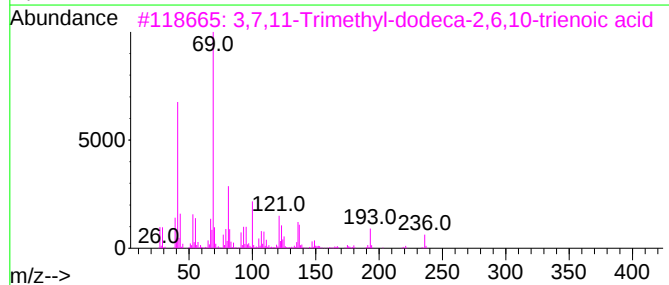
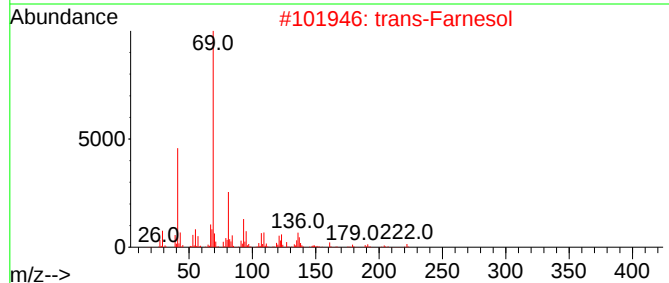
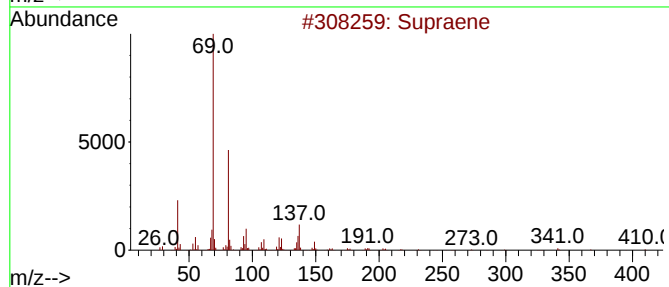
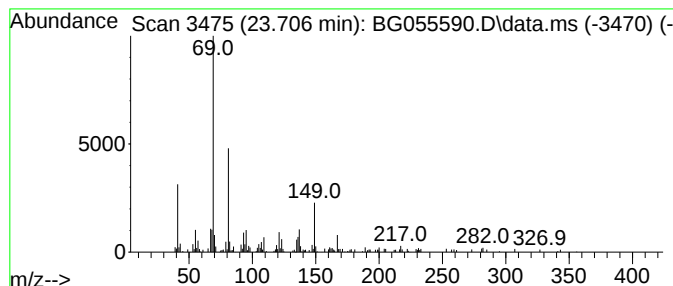
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.706	2.17 ng	168520	Perylene-d12	25.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	74
2			trans-Farnesol	222	C15H26O	000106-28-5	64
3			3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	53
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	53
5			(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055590.D
Acq On : 12 Nov 2022 15:11
Operator : CG/JU
Sample : N5431-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221170-COMP-05-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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
Butane, 2-metho...	3.324	43.9	ng	894539	1	8.271	407314	20.0
2-Pentanone, 4-...	5.321	3.7	ng	74920	1	8.271	407314	20.0
n-Hexadecanoic ...	18.488	7.2	ng	446634	4	17.630	1247170	20.0
Octadecanoic acid	19.746	3.1	ng	193913	4	17.630	1247170	20.0
1-Docosene	21.532	4.5	ng	316632	5	21.925	1403320	20.0
Supraene	23.706	2.2	ng	168520	6	25.357	1550040	20.0