

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022322\
 Data File : BM034061.D
 Acq On : 23 Feb 2022 20:18
 Operator : CG/JU
 Sample : N1627-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 20220092A-BERKELEY-4A-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_M\Methods\8270-BM022222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM034061.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.255	168	173	182	rBV	64218	98804	1.06%	0.181%
2	5.566	388	396	404	rBV	1311372	1920014	20.53%	3.524%
3	7.160	660	667	679	rVB	887428	1483788	15.87%	2.724%
4	8.019	805	813	820	rBV	700147	1128303	12.07%	2.071%
5	9.178	997	1010	1019	rBV	1678454	2751911	29.43%	5.051%
6	9.413	1044	1050	1057	rBV	86147	147813	1.58%	0.271%
7	10.607	1247	1253	1263	rBV	79694	134534	1.44%	0.247%
8	10.831	1283	1291	1298	rBV	895426	1479058	15.82%	2.715%
9	12.483	1567	1572	1580	rVB	70142	111104	1.19%	0.204%
10	13.283	1700	1708	1717	rBV	5004445	7296493	78.04%	13.393%
11	13.989	1821	1828	1834	rBV2	90694	139325	1.49%	0.256%
12	14.295	1874	1880	1887	rBV3	72612	121264	1.30%	0.223%
13	14.460	1901	1908	1916	rBV	59280	123865	1.32%	0.227%
14	14.648	1933	1940	1947	rBV	1373978	2049359	21.92%	3.762%
15	15.460	2072	2078	2084	rBV2	103992	155216	1.66%	0.285%
16	16.130	2185	2192	2199	rBV	4552871	6229795	66.63%	11.435%
17	17.318	2390	2394	2398	rBV	111820	126911	1.36%	0.233%
18	17.389	2400	2406	2412	rBV	1683710	2286141	24.45%	4.196%
19	17.677	2450	2455	2468	rBV	3935321	5061773	54.14%	9.291%
20	18.065	2517	2521	2526	rVB2	107020	137802	1.47%	0.253%
21	18.289	2554	2559	2568	rBV	901338	1351662	14.46%	2.481%
22	18.360	2568	2571	2578	rVB	130453	185532	1.98%	0.341%
23	19.565	2771	2776	2790	rBV	2803738	3923080	41.96%	7.201%
24	20.006	2845	2851	2861	rVB	8216522	9349961	100.00%	17.162%
25	20.653	2957	2961	2965	rBV	444010	517050	5.53%	0.949%
26	20.695	2965	2968	2973	rVB4	90769	123401	1.32%	0.227%
27	21.277	3063	3067	3072	rBV	437662	586193	6.27%	1.076%
28	21.559	3110	3115	3121	rBV	2007652	2646526	28.31%	4.858%
29	24.018	3527	3533	3547	rVB2	1313204	2813243	30.09%	5.164%

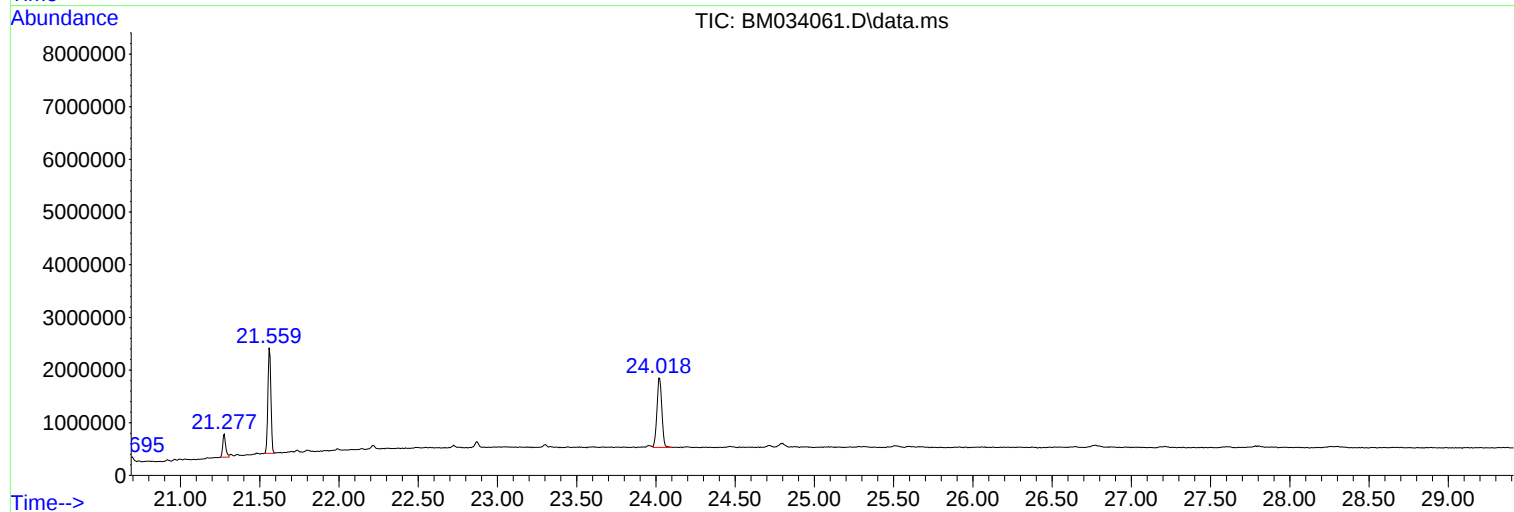
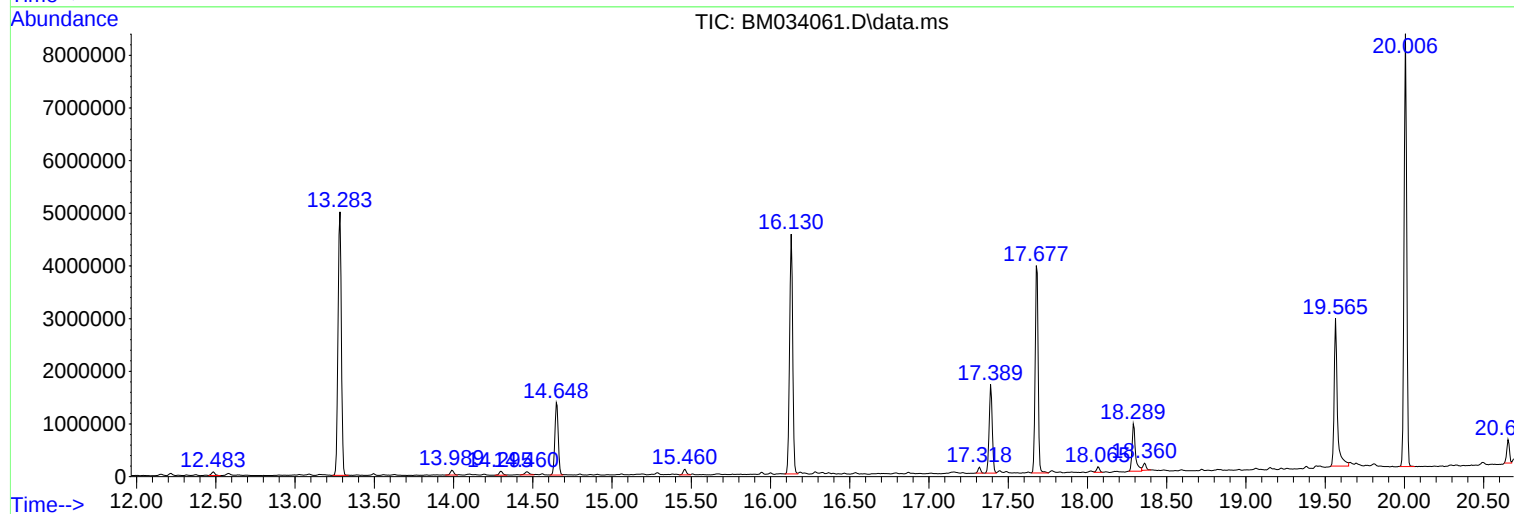
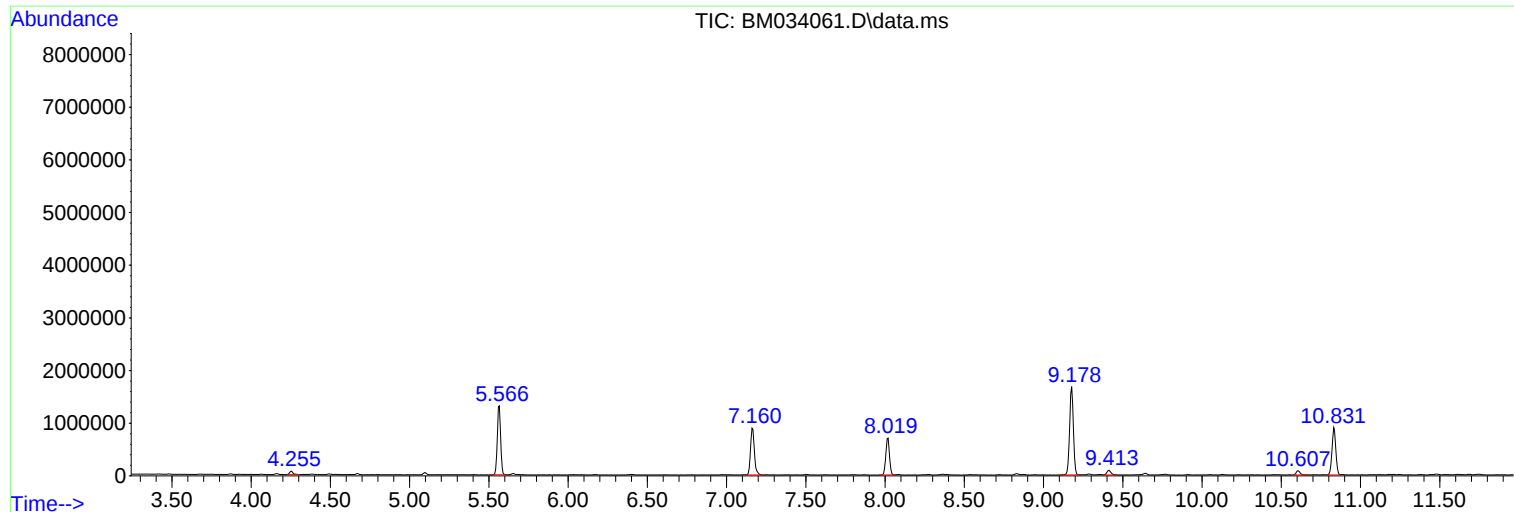
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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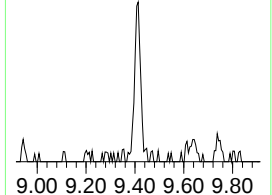
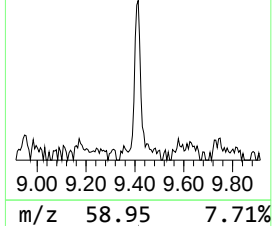
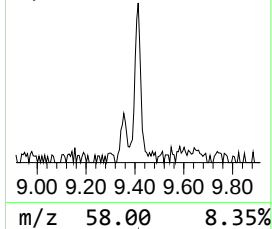
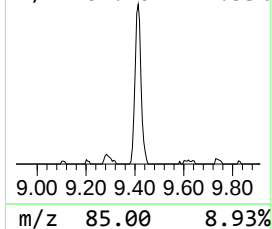
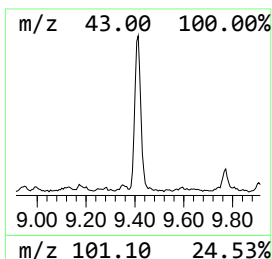
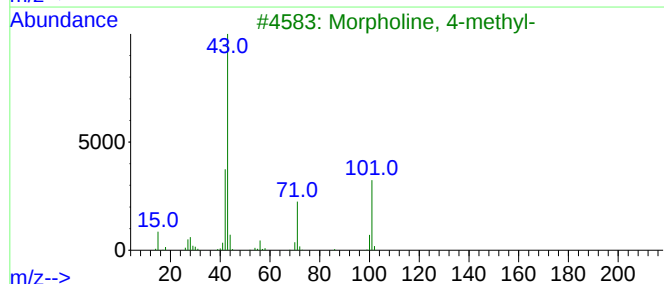
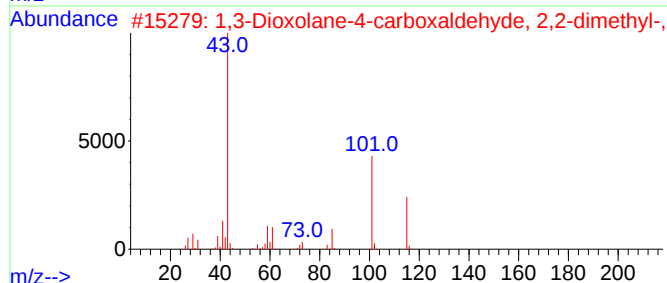
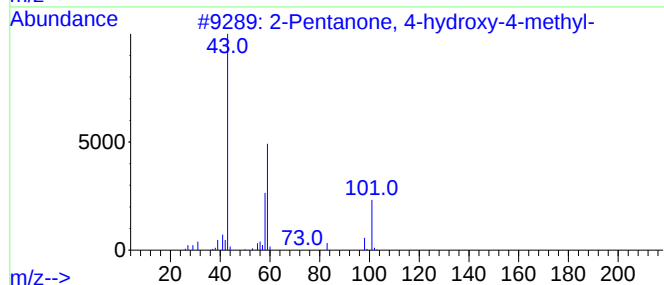
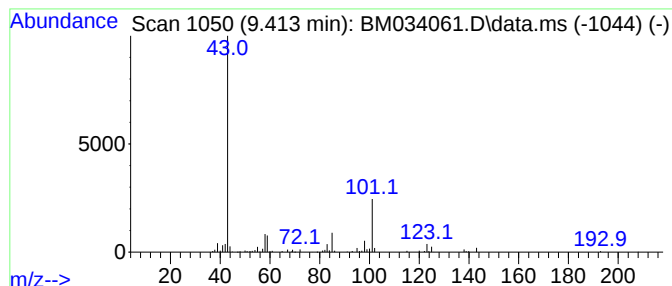
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.413	2.62 ng	147813	1,4-Dichlorobenzene-d4	8.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42		
2	1,3-Dioxolane-4-carboxaldehyde, ...	130	C6H10O3	015186-48-8	37		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	37		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
5	.alpha.-Hydroxyisobutyric acid, ...	146	C6H10O4	1000374-31-3	25		



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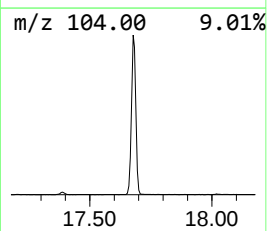
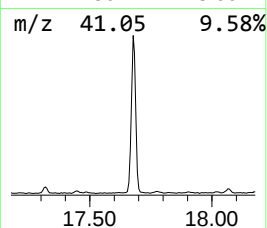
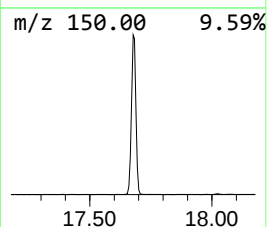
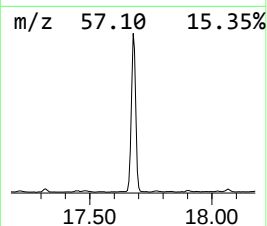
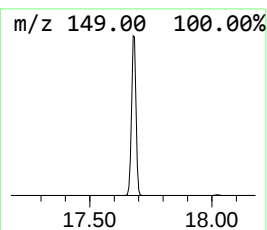
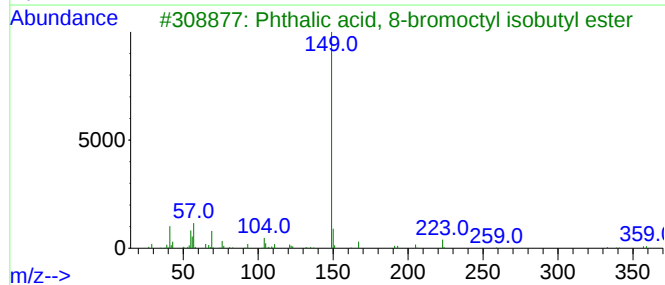
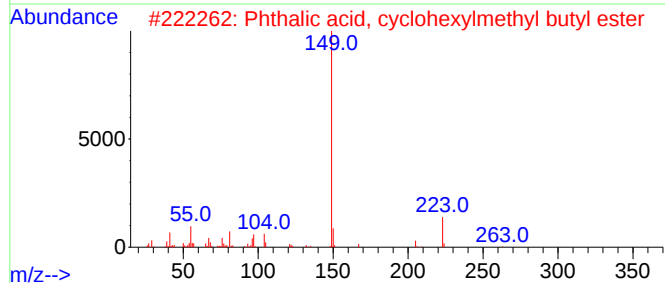
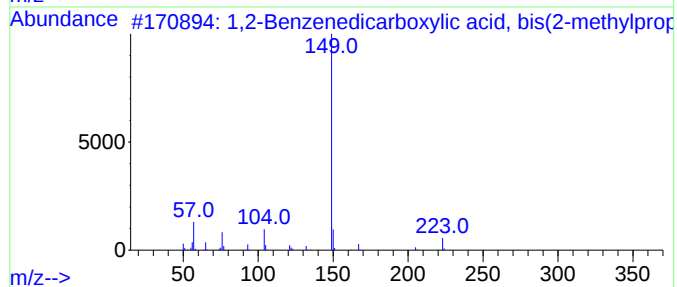
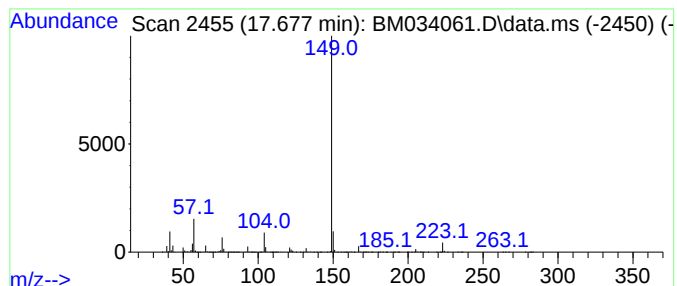
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Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.677	44.28 ng	5061770	Phenanthrene-d10	17.389

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2			Phthalic acid, cyclohexylmethyl ...	318	C19H26O4	1000309-08-6	78
3			Phthalic acid, 8-bromooctyl isobu...	412	C20H29BrO4	1000382-55-3	78
4			Phthalic acid, isobutyl 2-propyl...	334	C20H30O4	1000377-91-9	78
5			Phthalic acid, isobutyl octyl ester	334	C20H30O4	1010309-04-5	78



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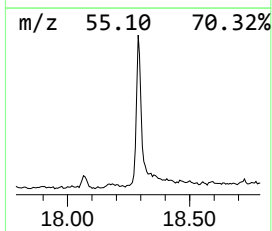
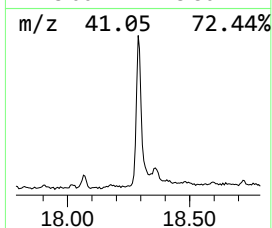
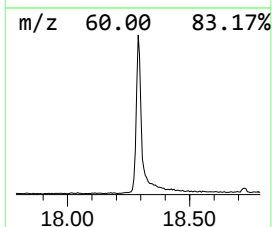
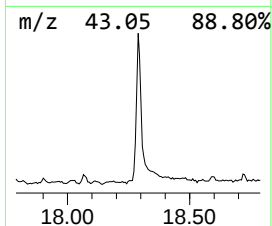
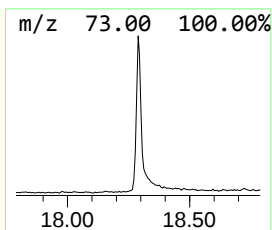
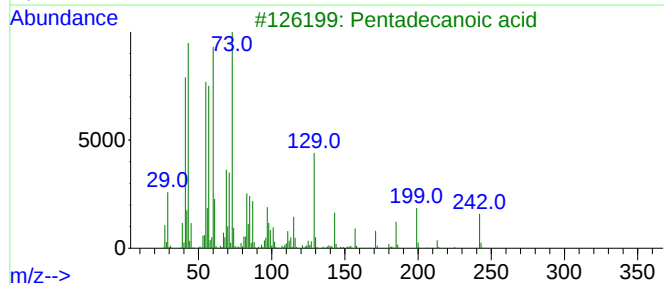
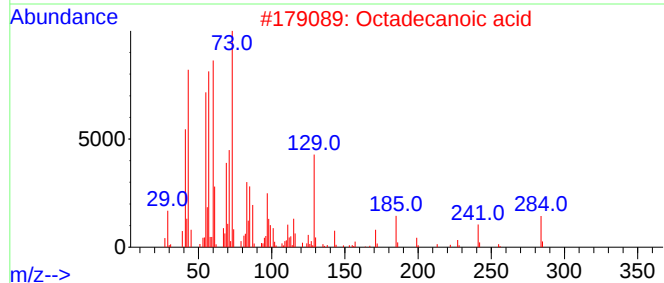
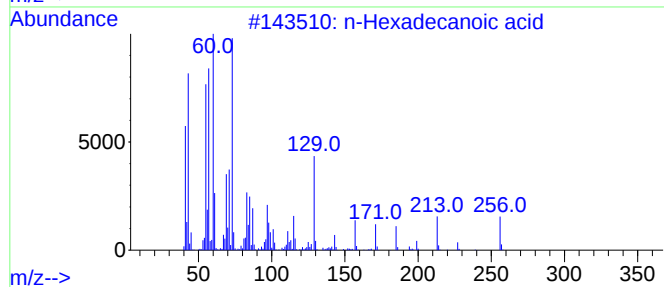
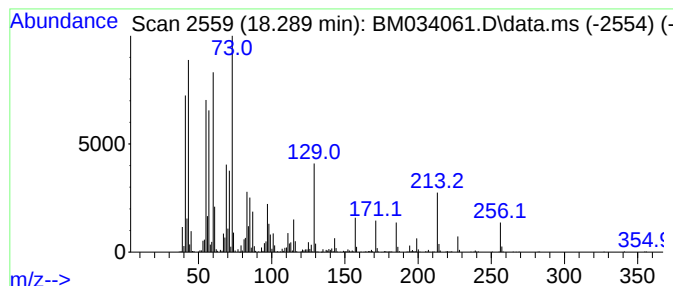
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.289	11.82 ng	1351660	Phenanthrene-d10	17.389

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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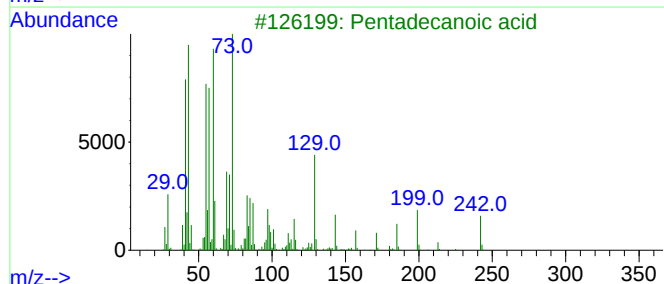
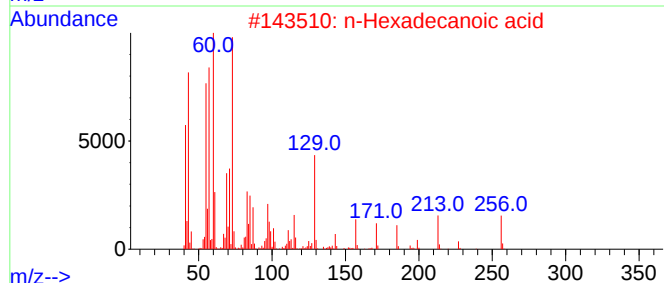
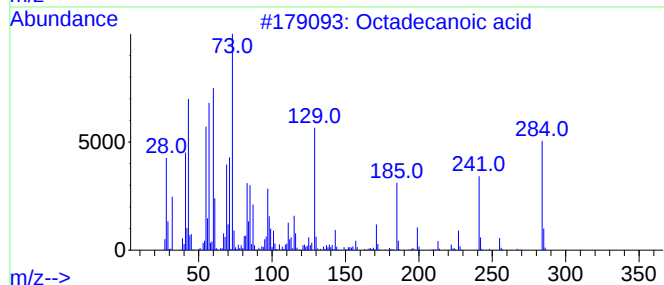
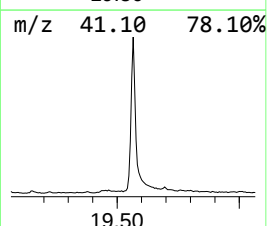
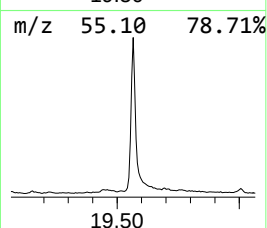
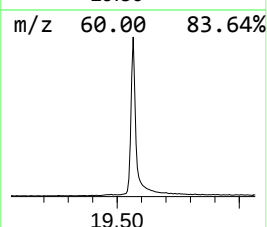
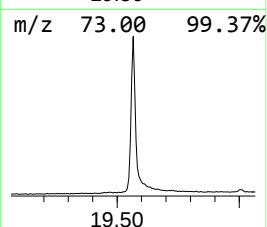
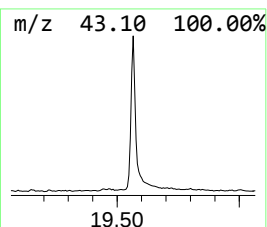
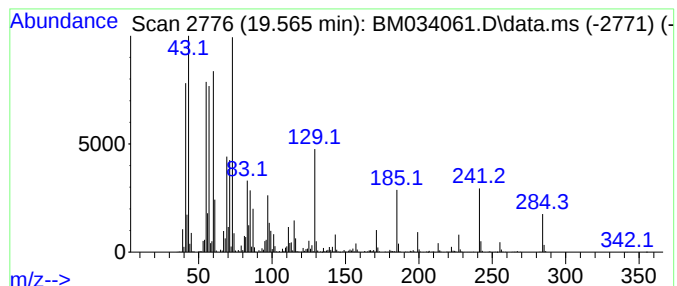
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.565	29.65 ng	3923080	Chrysene-d12	21.559

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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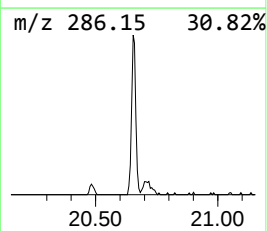
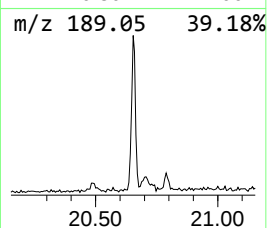
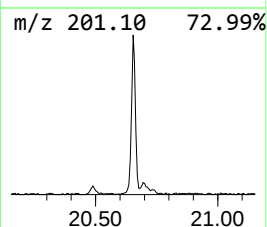
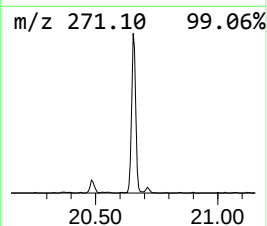
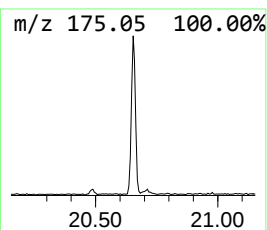
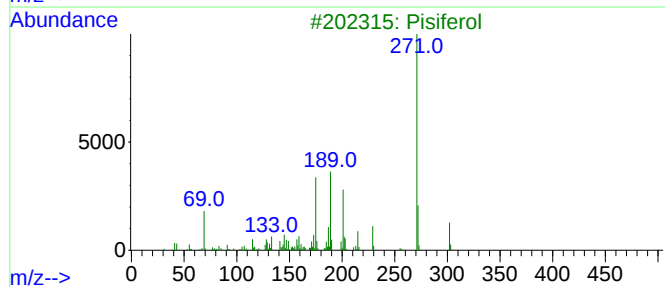
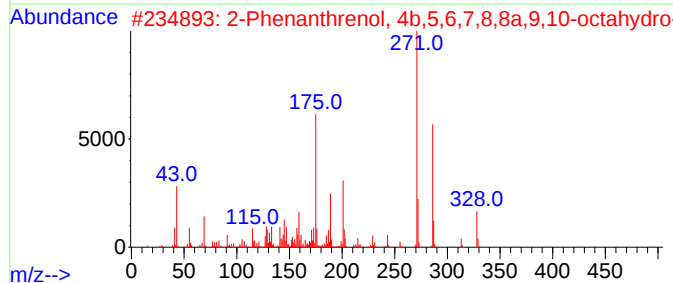
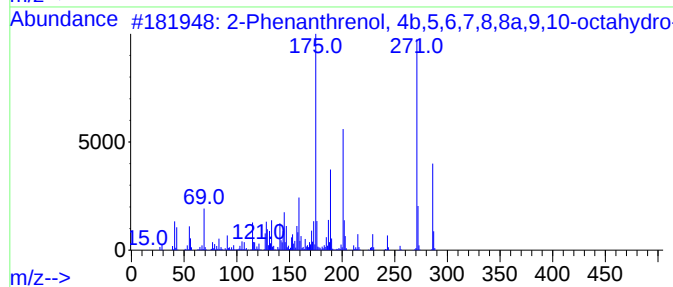
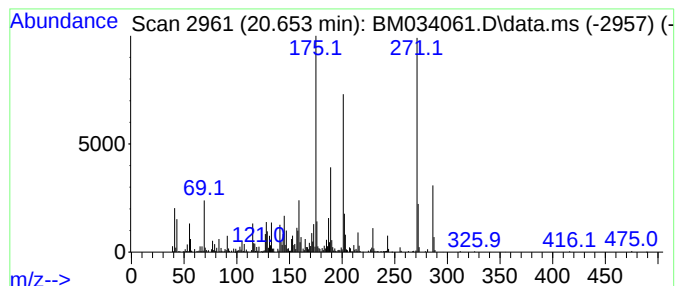
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Peak Number 5 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.654	3.91 ng	517050	Chrysene-d12	21.559

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H300	000511-15-9	99		
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H3202	015340-82-6	90		
3	Pisiferol	302	C20H3002	024035-36-7	47		
4	(4Br,8As)-(+)-4B,5,6,7,8,8A,9,10...	346	C22H3403	1000426-72-2	46		
5	13-Isopropylpodocarpin-12-ol-20-a1	300	C20H2802	024035-37-8	46		



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ClientSampleId :
20220092A-BERKELEY-4A-ELUTRIATE

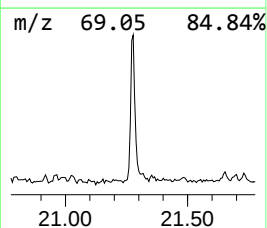
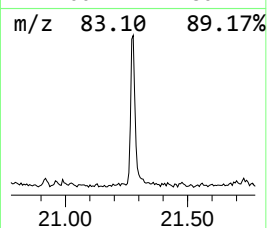
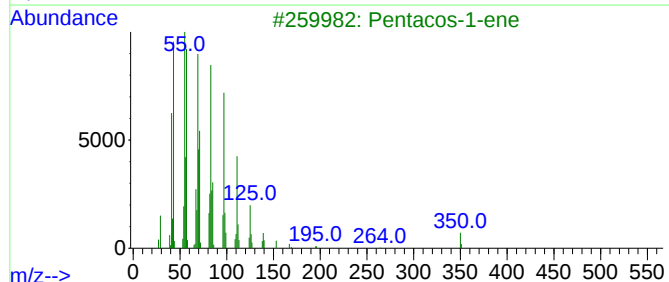
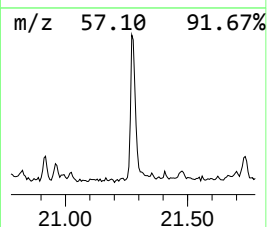
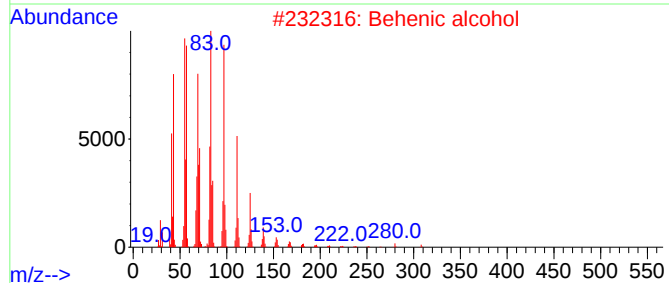
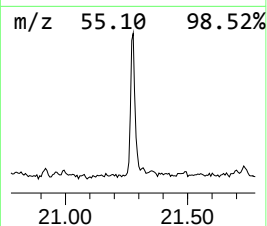
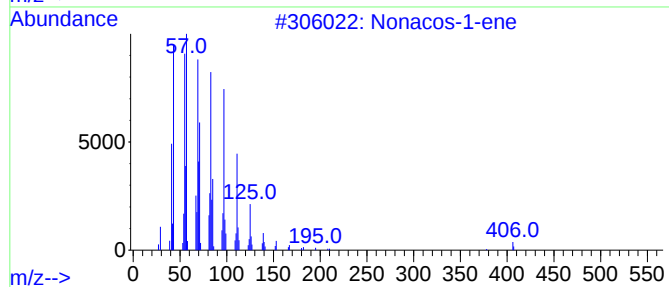
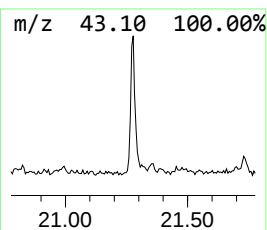
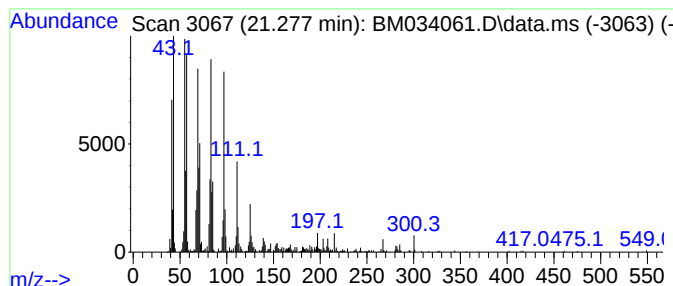
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonacos-1-ene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.277	4.43 ng	586193	Chrysene-d12	21.559

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacos-1-ene	406	C29H58	018835-35-3	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022322\
Data File : BM034061.D
Acq On : 23 Feb 2022 20:18
Operator : CG/JU
Sample : N1627-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20220092A-BERKELEY-4A-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.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-...	9.413	2.6	ng	147813	1	8.019	1128300	20.0
1,2-Benzenedica...	17.677	44.3	ng	5061770	4	17.389	2286140	20.0
n-Hexadecanoic ...	18.289	11.8	ng	1351660	4	17.389	2286140	20.0
Octadecanoic acid	19.565	29.6	ng	3923080	5	21.559	2646530	20.0
2-Phenanthrenol...	20.654	3.9	ng	517050	5	21.559	2646530	20.0
Nonacos-1-ene	21.277	4.4	ng	586193	5	21.559	2646530	20.0