

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
 Data File : BM047254.D
 Acq On : 19 Aug 2024 16:08
 Operator : RC/JU
 Sample : P3580-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 926-K1-SD-0-0.5-081224

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047254.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.264	60	64	75	rBV	87195	139796	2.63%	0.344%
2	4.569	282	286	296	rVB	79421	120085	2.26%	0.296%
3	5.022	356	363	378	rBV	1753131	2717656	51.22%	6.693%
4	6.581	621	628	638	rBV	1770343	2856492	53.83%	7.035%
5	7.363	755	761	770	rVB	594986	898039	16.92%	2.212%
6	7.663	807	812	819	rVB	69667	107067	2.02%	0.264%
7	8.510	947	956	967	rBV	1147749	1843114	34.74%	4.539%
8	9.093	1050	1055	1060	rBV	45190	67363	1.27%	0.166%
9	10.122	1221	1230	1237	rBV	732564	1224649	23.08%	3.016%
10	10.881	1353	1359	1370	rBV	136798	269487	5.08%	0.664%
11	12.628	1650	1656	1668	rBV	2357326	3619322	68.21%	8.914%
12	13.910	1862	1874	1887	rBV3	65161	232524	4.38%	0.573%
13	14.022	1887	1893	1902	rVB	1181149	1742664	32.84%	4.292%
14	14.280	1929	1937	1945	rVB2	82239	182736	3.44%	0.450%
15	14.492	1969	1973	1982	rVB7	27963	56300	1.06%	0.139%
16	14.880	2032	2039	2045	rBV	72837	127934	2.41%	0.315%
17	15.533	2144	2150	2163	rVV	2843789	4030401	75.96%	9.926%
18	16.792	2358	2364	2369	rBV	1555940	2212831	41.70%	5.450%
19	16.998	2395	2399	2407	rBV9	45230	99034	1.87%	0.244%
20	17.557	2491	2494	2501	rVB8	39533	65348	1.23%	0.161%
21	17.692	2513	2517	2518	rBV2	79801	94855	1.79%	0.234%
22	17.727	2518	2523	2530	rVV	920925	1478694	27.87%	3.642%
23	17.786	2531	2533	2539	rVB	112843	164757	3.11%	0.406%
24	18.268	2611	2615	2620	rBV	45327	68114	1.28%	0.168%
25	18.868	2714	2717	2720	rBV	69119	100734	1.90%	0.248%
26	19.027	2739	2744	2767	rBV	2191490	3752982	70.73%	9.243%
27	19.280	2784	2787	2796	rVB2	94522	166637	3.14%	0.410%
28	19.457	2812	2817	2825	rVB	4311660	5306055	100.00%	13.068%
29	20.768	3036	3040	3047	rBV	568085	829859	15.64%	2.044%
30	21.033	3080	3085	3090	rBV	2081559	2868354	54.06%	7.064%
31	23.733	3538	3544	3560	rVB	1355438	3160332	59.56%	7.783%

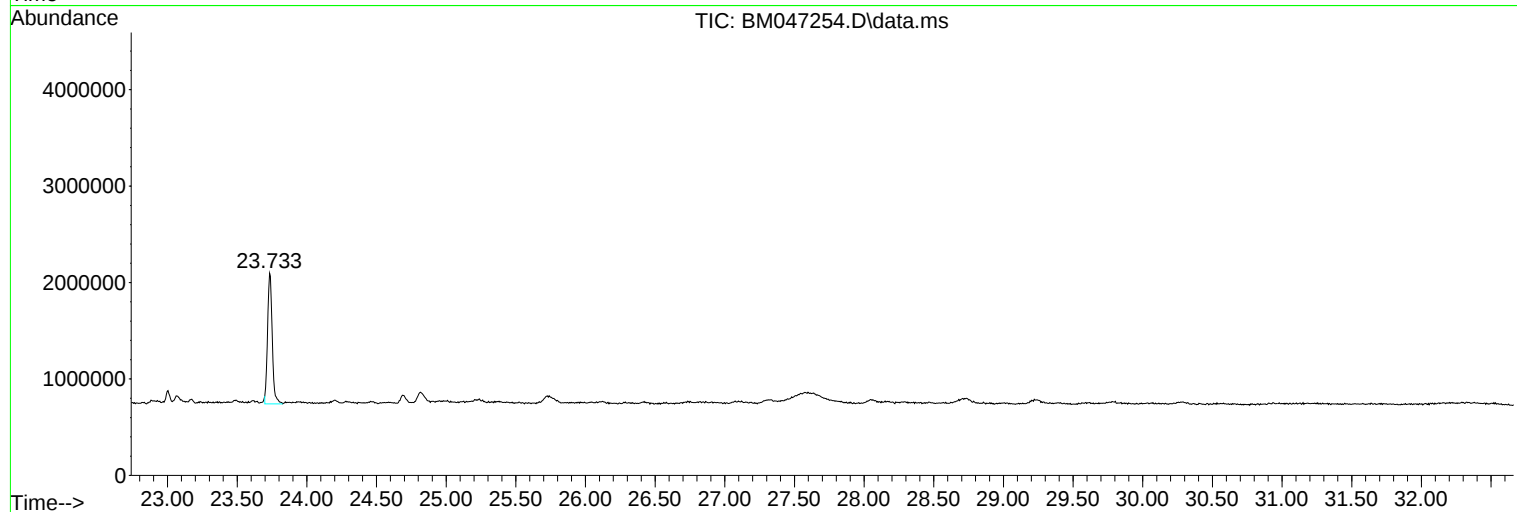
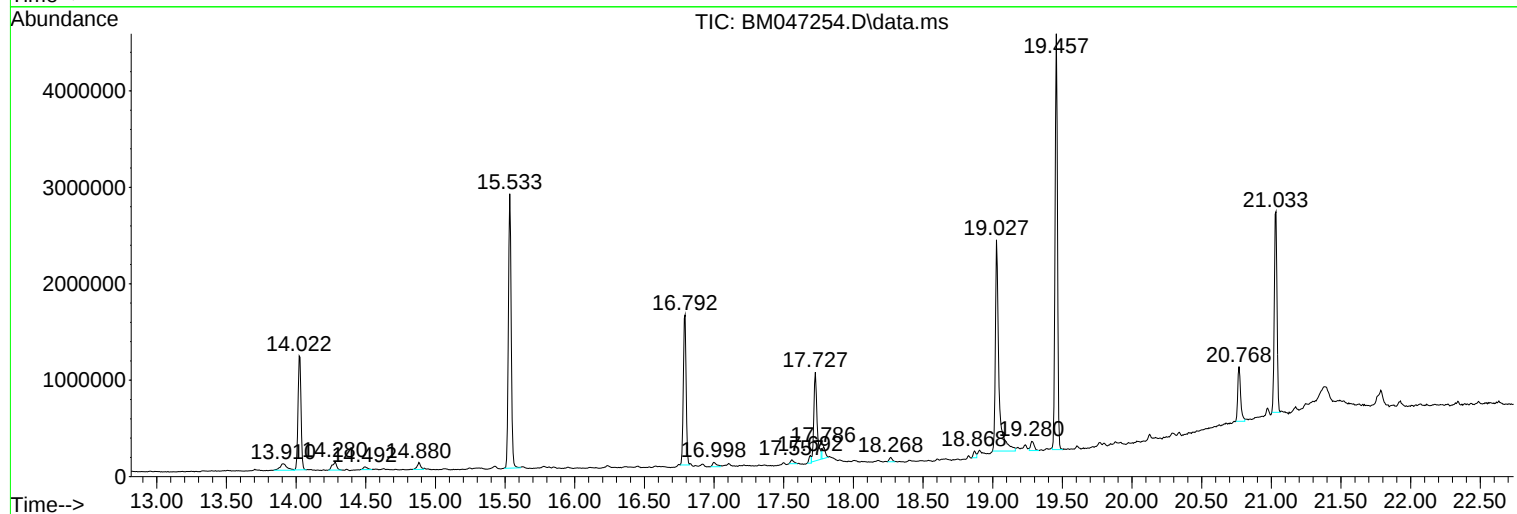
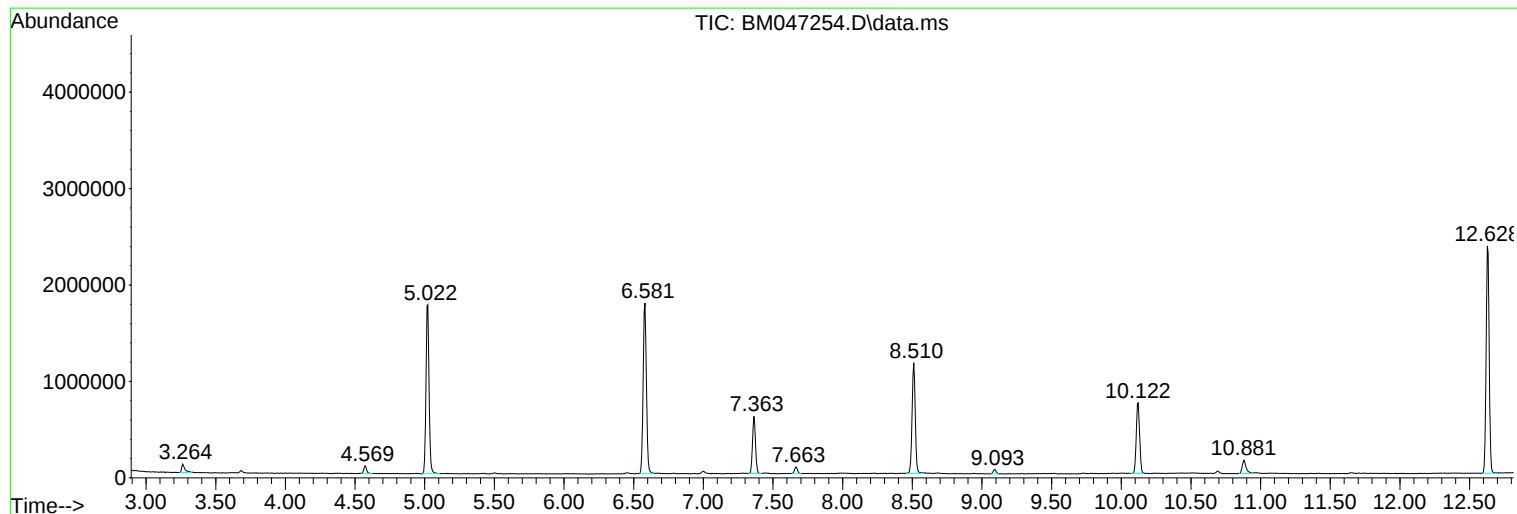
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926-K1-SD-0-0.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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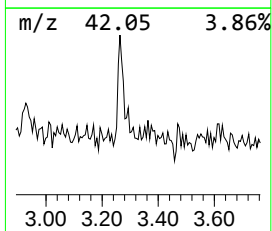
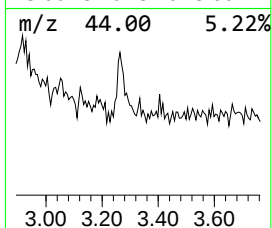
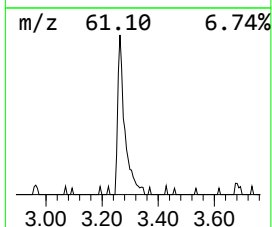
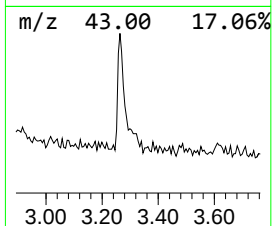
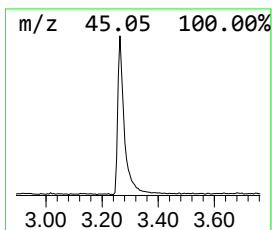
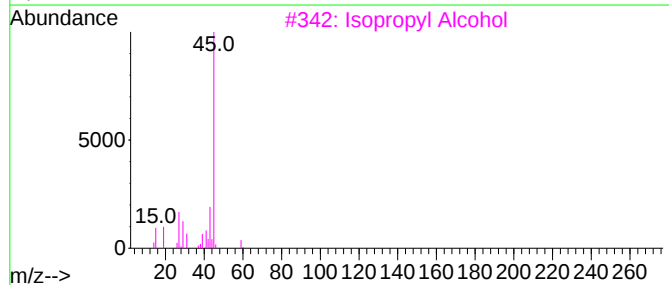
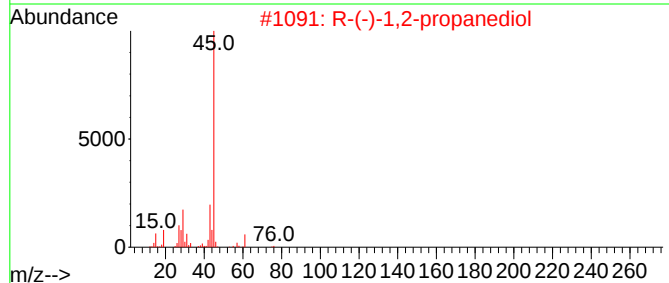
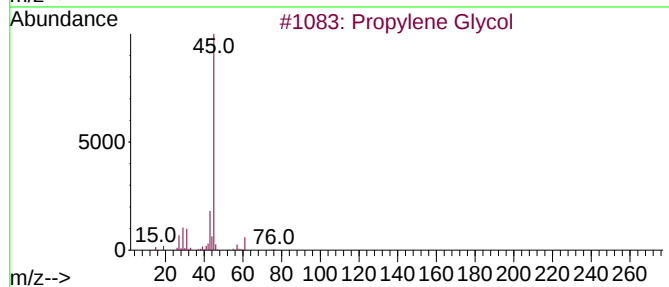
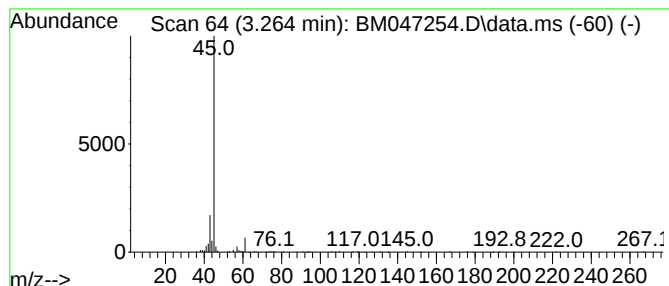
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.264	3.11 ng	139796	1,4-Dichlorobenzene-d4	7.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	10



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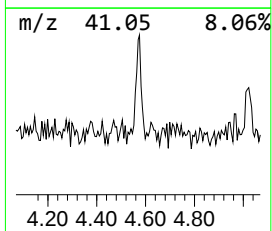
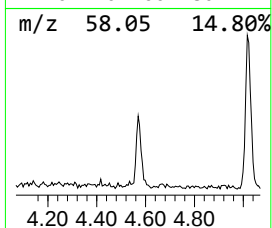
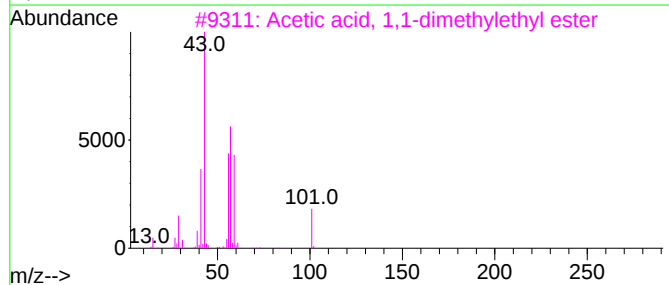
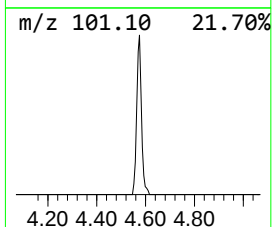
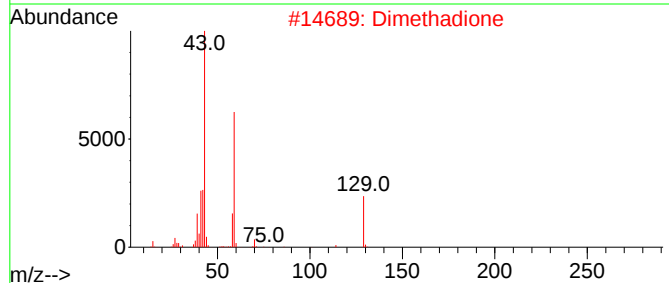
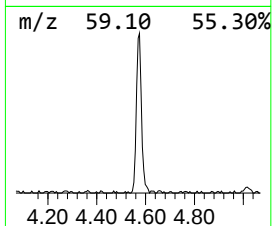
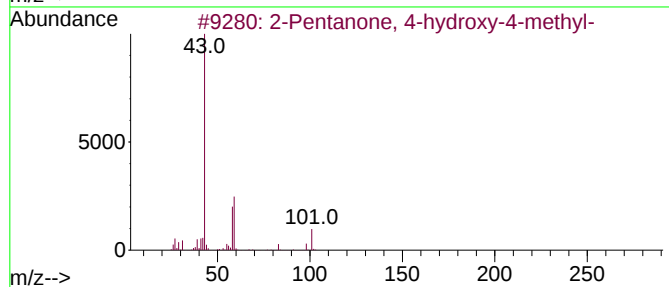
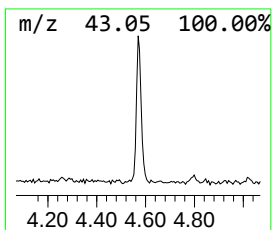
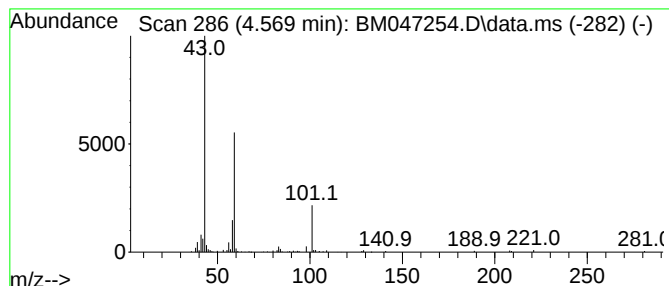
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	2.67 ng	120085	1,4-Dichlorobenzene-d4	7.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Dimethadione	129	C5H7NO3	000695-53-4	40		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
5	Propanoic acid, 3-nitro-, methyl...	133	C4H7NO4	020497-95-4	17		



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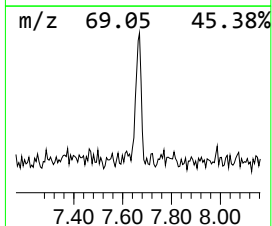
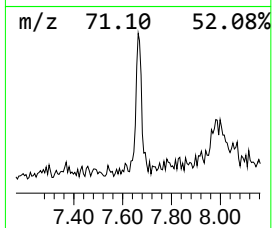
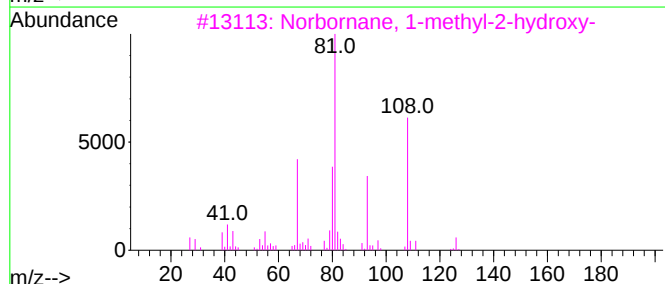
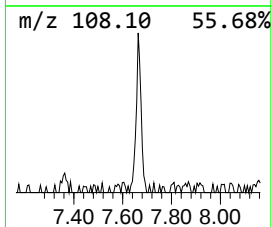
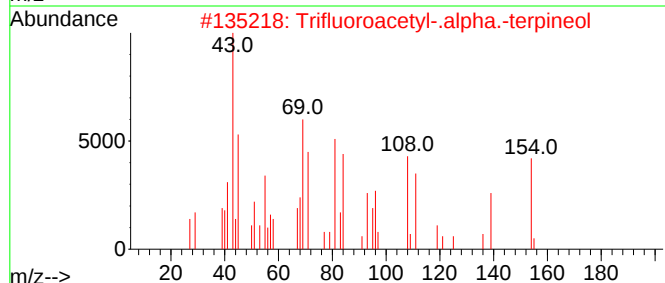
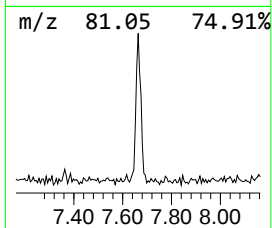
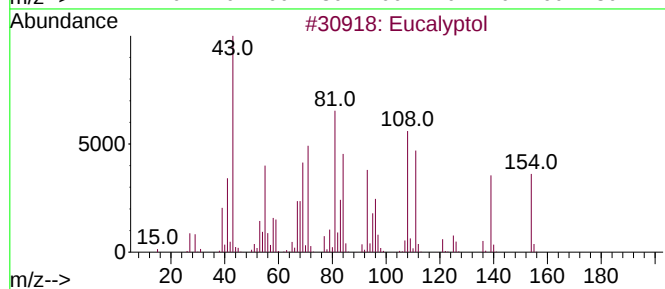
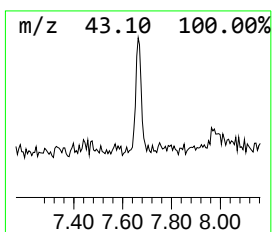
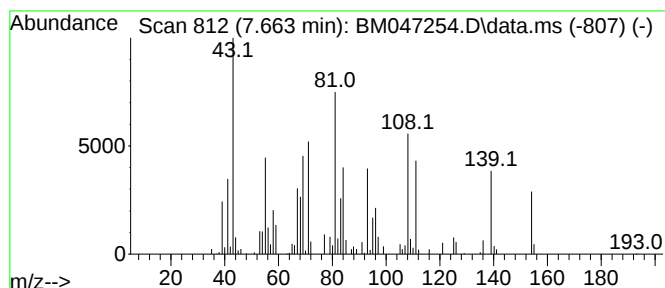
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Eucalyptol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.663	2.38 ng	107067	1,4-Dichlorobenzene-d4	7.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	98
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	38
3			Norbornane, 1-methyl-2-hydroxy-	126	C8H14O	054339-50-3	27
4			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	25
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	18



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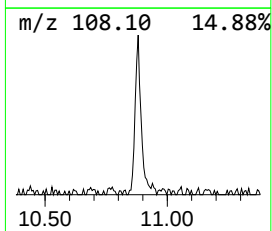
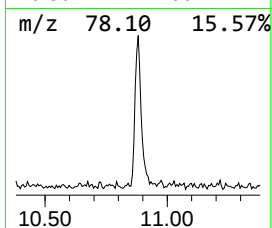
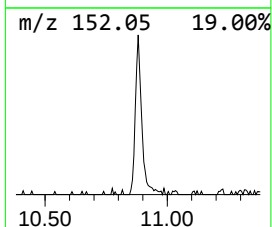
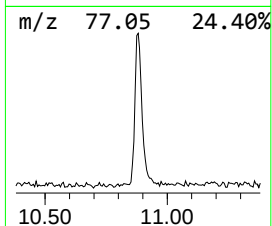
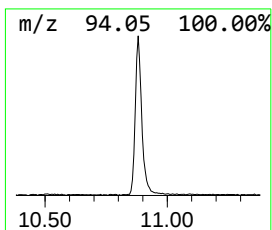
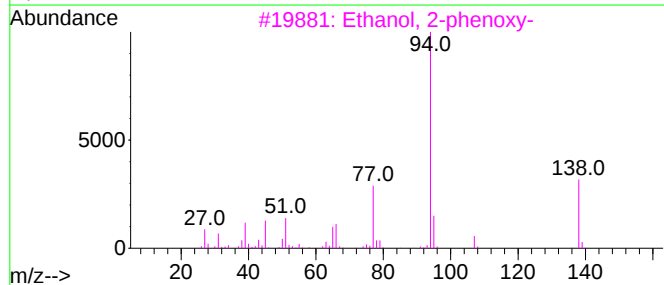
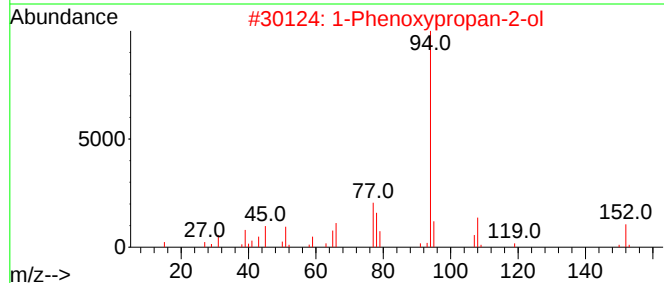
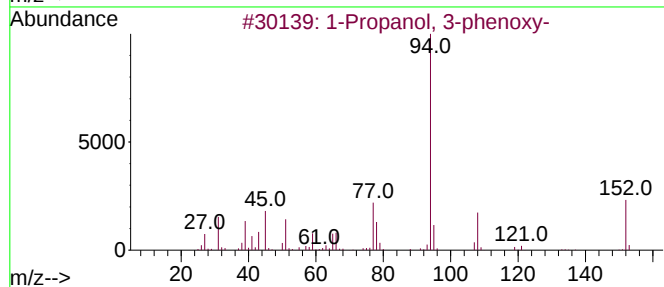
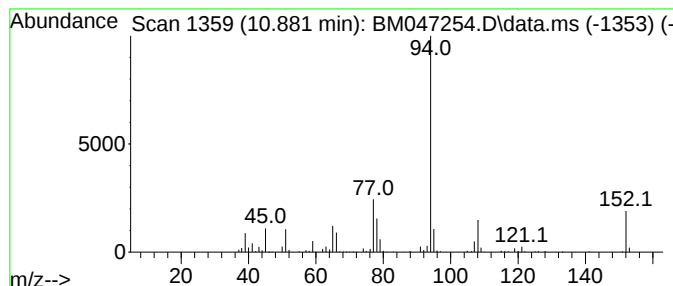
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Propanol, 3-phenoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	4.40 ng	269487	Naphthalene-d8	10.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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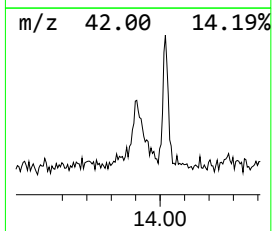
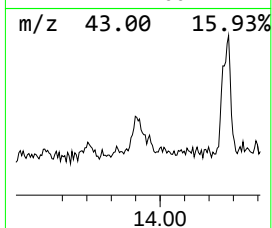
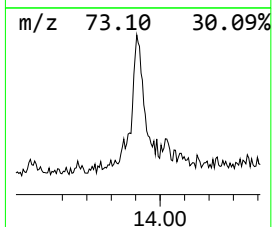
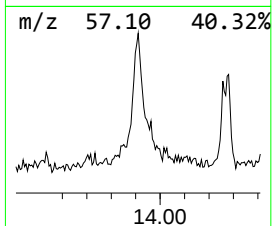
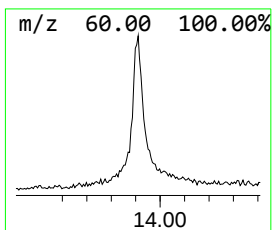
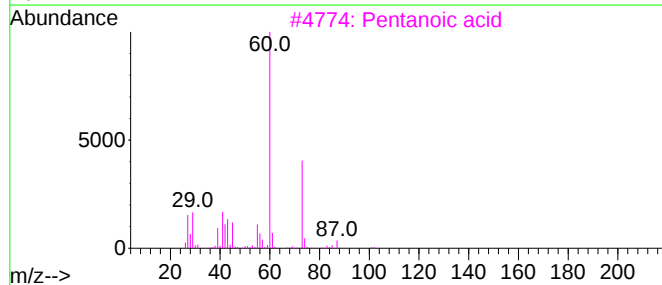
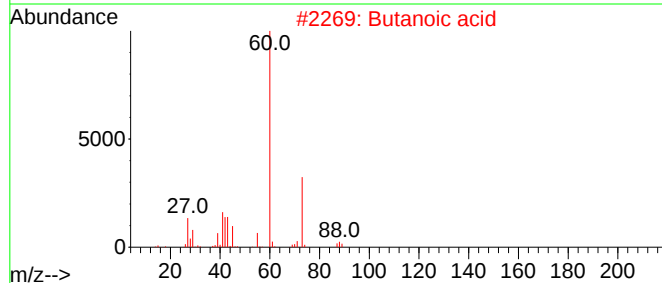
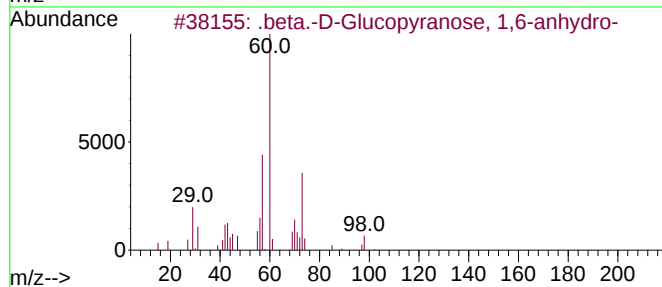
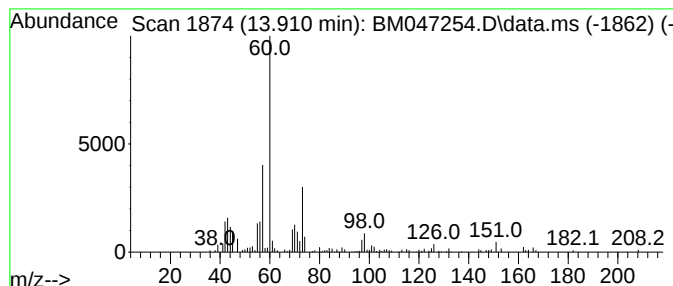
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 .beta.-D-Glucopyranose, 1,6... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	2.67 ng	232524	Acenaphthene-d10	14.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	72
2			Butanoic acid	88	C4H8O2	000107-92-6	53
3			Pentanoic acid	102	C5H10O2	000109-52-4	53
4			D-Allose	180	C6H12O6	002595-97-3	49
5			Heptanoic acid	130	C7H14O2	000111-14-8	45



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ClientSampleId :
926-K1-SD-0-0.5-081224

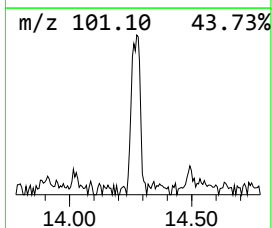
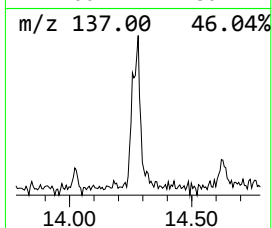
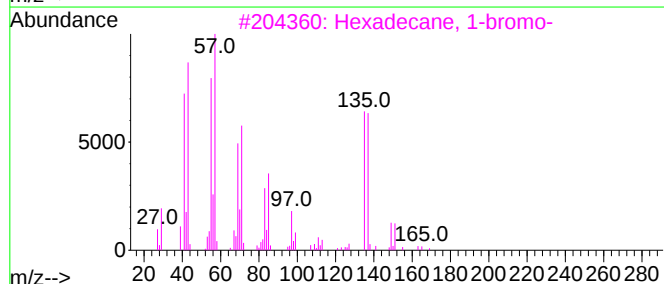
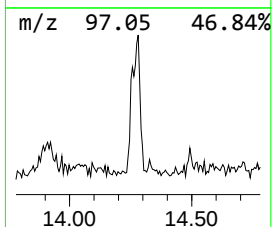
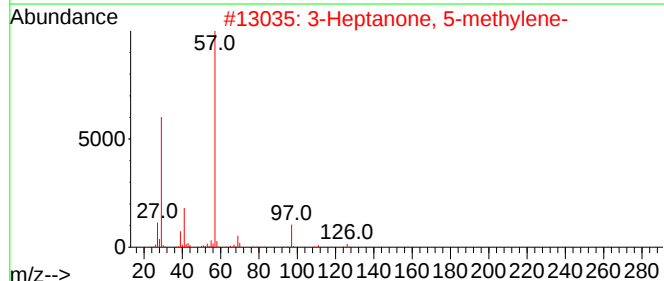
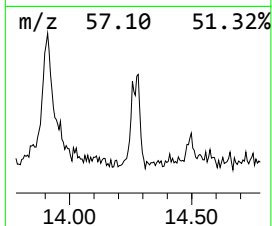
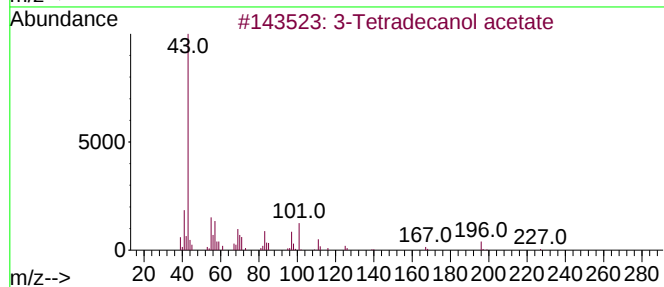
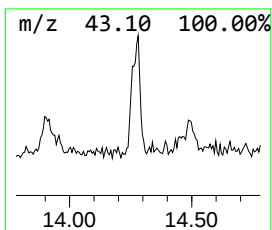
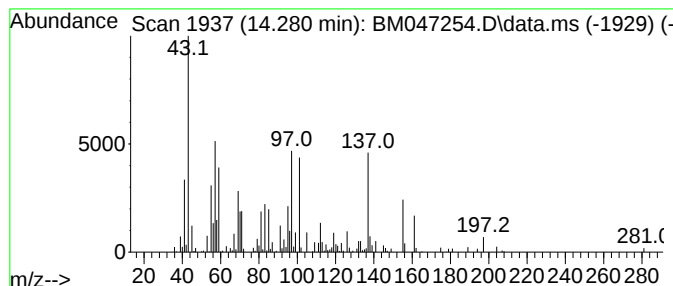
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.281 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.281	2.10 ng	182736	Acenaphthene-d10	14.028

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	14	
2	3-Heptanone, 5-methylene-	126	C8H14O	020690-70-4	10	
3	Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	9	
4	Undecane, 1-bromo-	234	C11H23Br	000693-67-4	9	
5	E-8-Methyl-7-dodecen-1-ol acetate	240	C15H28O2	1000131-32-2	9	



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047254.D
Acq On : 19 Aug 2024 16:08
Operator : RC/JU
Sample : P3580-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

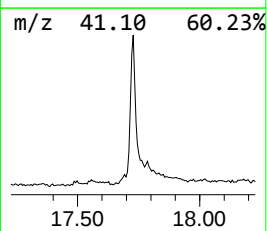
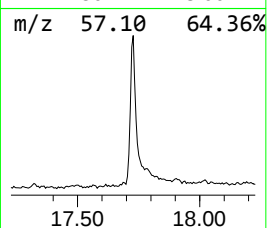
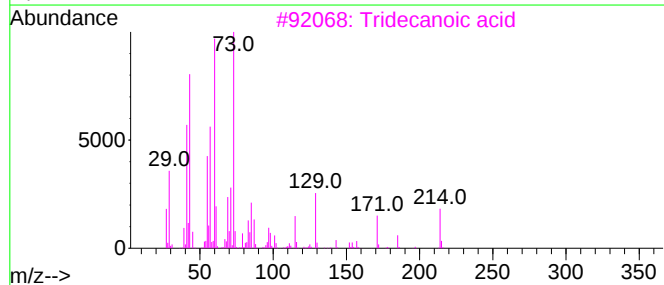
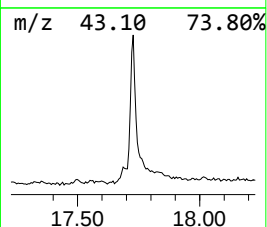
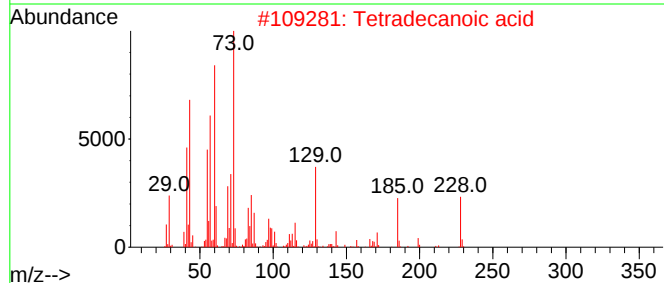
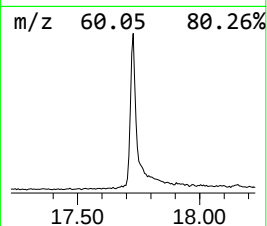
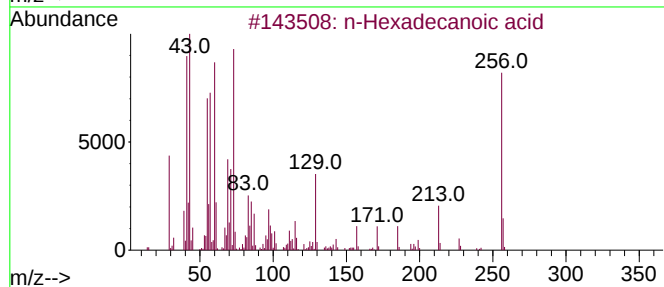
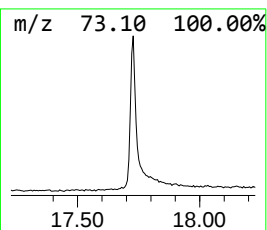
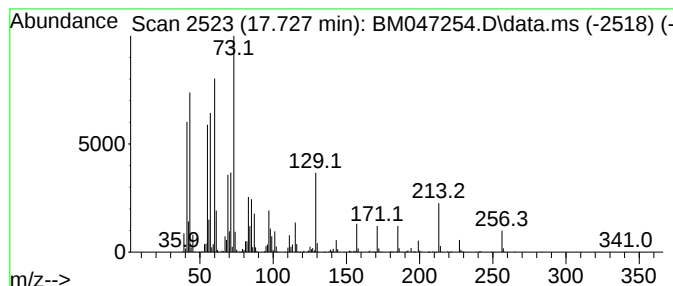
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ClientSampleId :
926-K1-SD-0-0.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.727	13.36 ng	1478690	Phenanthrene-d10	16.792	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047254.D
Acq On : 19 Aug 2024 16:08
Operator : RC/JU
Sample : P3580-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
926-K1-SD-0-0.5-081224

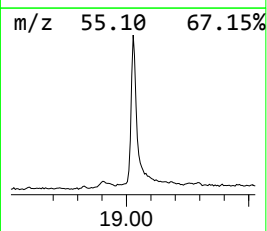
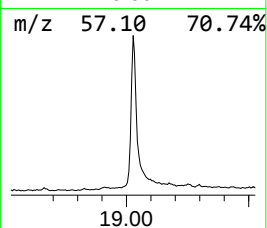
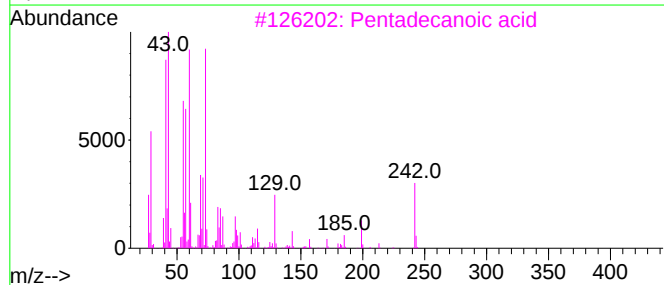
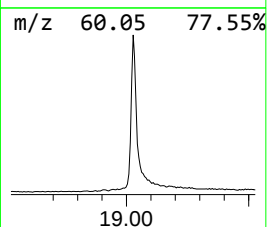
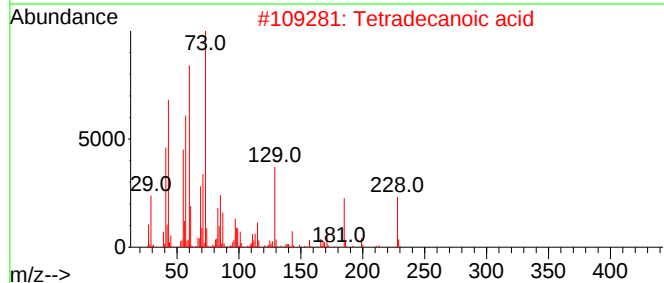
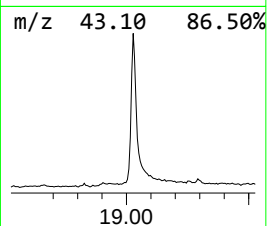
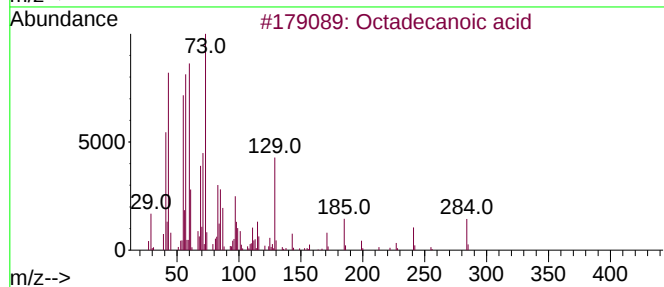
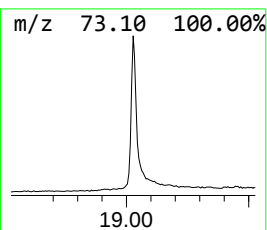
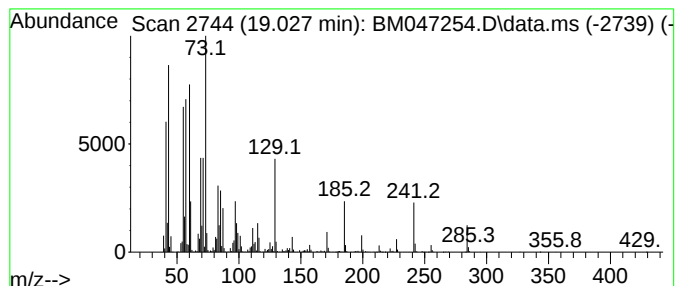
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.027	26.17 ng	3752980	Chrysene-d12	21.033

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	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047254.D
Acq On : 19 Aug 2024 16:08
Operator : RC/JU
Sample : P3580-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
926-K1-SD-0-0.5-081224

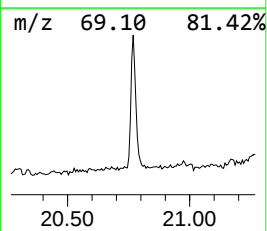
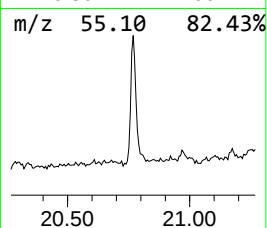
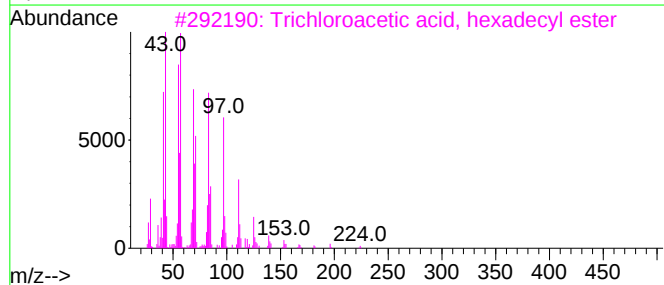
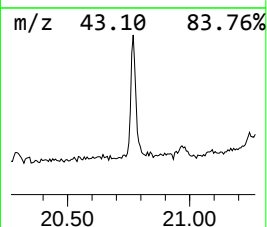
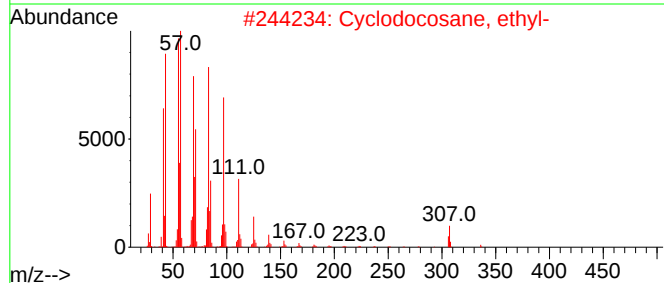
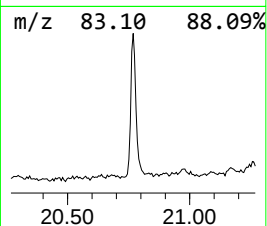
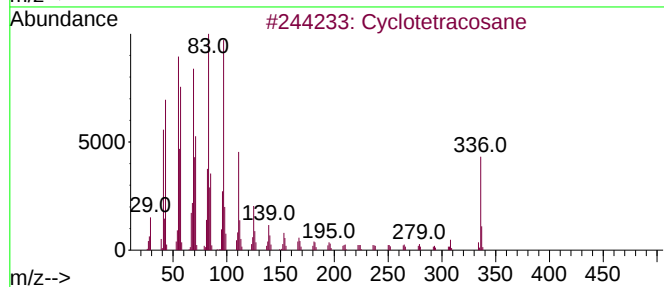
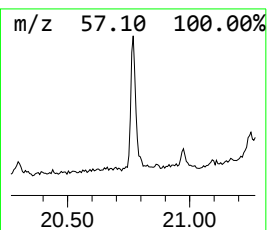
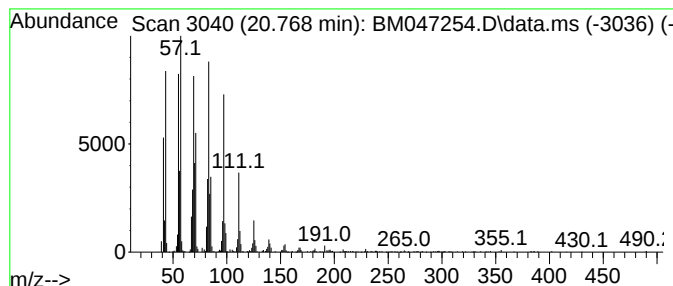
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.768	5.79 ng	829859	Chrysene-d12	21.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	94
2			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			1-Hexacosanol	382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047254.D
Acq On : 19 Aug 2024 16:08
Operator : RC/JU
Sample : P3580-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
926-K1-SD-0-0.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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
Propylene Glycol	3.264	3.1	ng	139796	1	7.363	898039	20.0
2-Pentanone, 4-...	4.569	2.7	ng	120085	1	7.363	898039	20.0
Eucalyptol	7.663	2.4	ng	107067	1	7.363	898039	20.0
1-Propanol, 3-p...	10.881	4.4	ng	269487	2	10.122	1224650	20.0
.beta.-D-Glucop...	13.910	2.7	ng	232524	3	14.028	1742660	20.0
unknown14.281	14.281	2.1	ng	182736	3	14.028	1742660	20.0
n-Hexadecanoic ...	17.727	13.4	ng	1478690	4	16.792	2212830	20.0
Octadecanoic acid	19.027	26.2	ng	3752980	5	21.033	2868350	20.0
Cyclotetracosane	20.768	5.8	ng	829859	5	21.033	2868350	20.0