

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
 Data File : BM029729.D
 Acq On : 30 Apr 2021 14:57
 Operator : CG/JU
 Sample : M2207-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-6A-5-COMP

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-BM043021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029729.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.193	385	392	404	rBV	952801	1336136	30.23%	6.350%
2	6.781	655	662	677	rBV	849809	1384867	31.33%	6.582%
3	7.587	793	799	806	rBV	200565	311637	7.05%	1.481%
4	8.746	989	996	1007	rBV	565968	916445	20.74%	4.356%
5	10.369	1264	1272	1279	rBV	243947	413456	9.35%	1.965%
6	12.851	1687	1694	1705	rBV	1768458	2576736	58.30%	12.247%
7	13.139	1738	1743	1750	rVB	27379	46608	1.05%	0.222%
8	13.698	1833	1838	1846	rVB	105940	149742	3.39%	0.712%
9	14.233	1924	1929	1937	rVB	405823	603463	13.65%	2.868%
10	15.733	2178	2184	2192	rVB	1547448	2205778	49.91%	10.484%
11	16.033	2230	2235	2243	rVB2	32281	60336	1.37%	0.287%
12	16.292	2274	2279	2283	rBV	29491	52208	1.18%	0.248%
13	16.386	2289	2295	2307	rVB3	132104	324101	7.33%	1.540%
14	16.892	2375	2381	2391	rVV	41174	139304	3.15%	0.662%
15	16.980	2391	2396	2401	rVV	517658	748475	16.94%	3.557%
16	17.022	2401	2403	2410	rVB	44530	56996	1.29%	0.271%
17	17.892	2546	2551	2561	rBV	466645	627923	14.21%	2.984%
18	18.168	2590	2598	2601	rBV	227067	400498	9.06%	1.903%
19	18.216	2601	2606	2616	rVB	402300	729688	16.51%	3.468%
20	19.045	2741	2747	2755	rBV	94353	175250	3.97%	0.833%
21	19.174	2765	2769	2779	rBV	208704	301016	6.81%	1.431%
22	19.404	2800	2808	2813	rBV	78360	135994	3.08%	0.646%
23	19.615	2839	2844	2849	rBV	3587109	4419659	100.00%	21.006%
24	19.910	2891	2894	2898	rVB2	45667	58299	1.32%	0.277%
25	20.892	3057	3061	3067	rBV	231607	313335	7.09%	1.489%
26	21.168	3102	3108	3112	rBV	818557	1069379	24.20%	5.083%
27	21.651	3185	3190	3197	rBV	103570	264763	5.99%	1.258%
28	22.192	3279	3282	3288	rVB2	134396	184983	4.19%	0.879%
29	23.339	3471	3477	3485	rBV2	571726	1033026	23.37%	4.910%

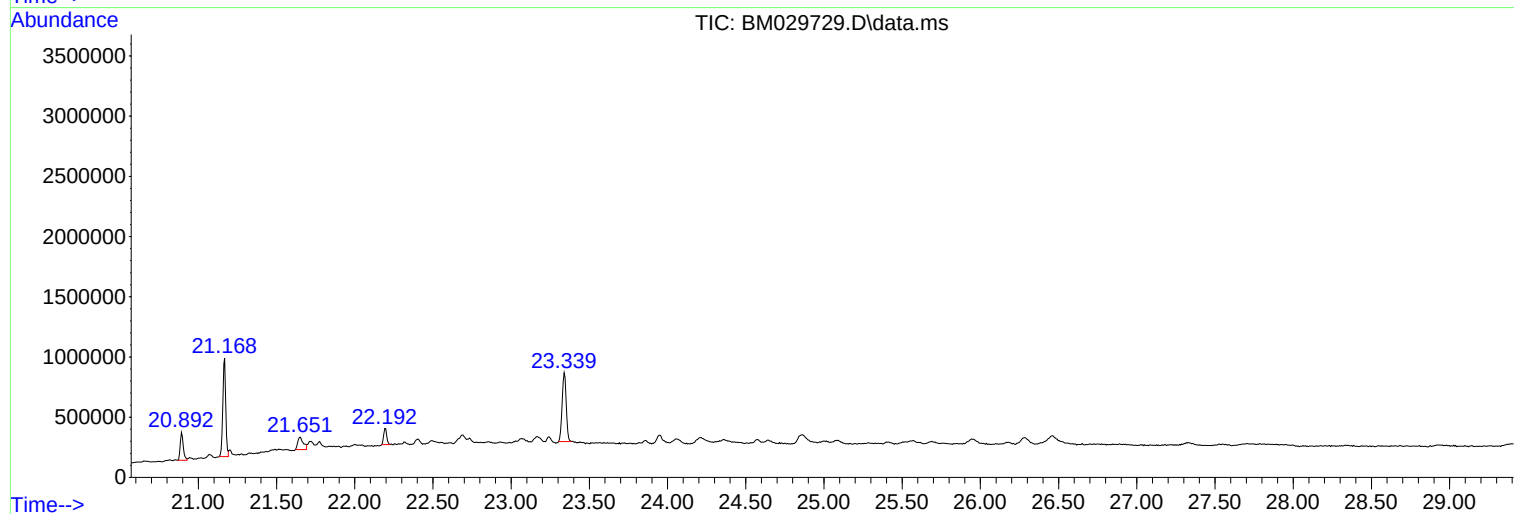
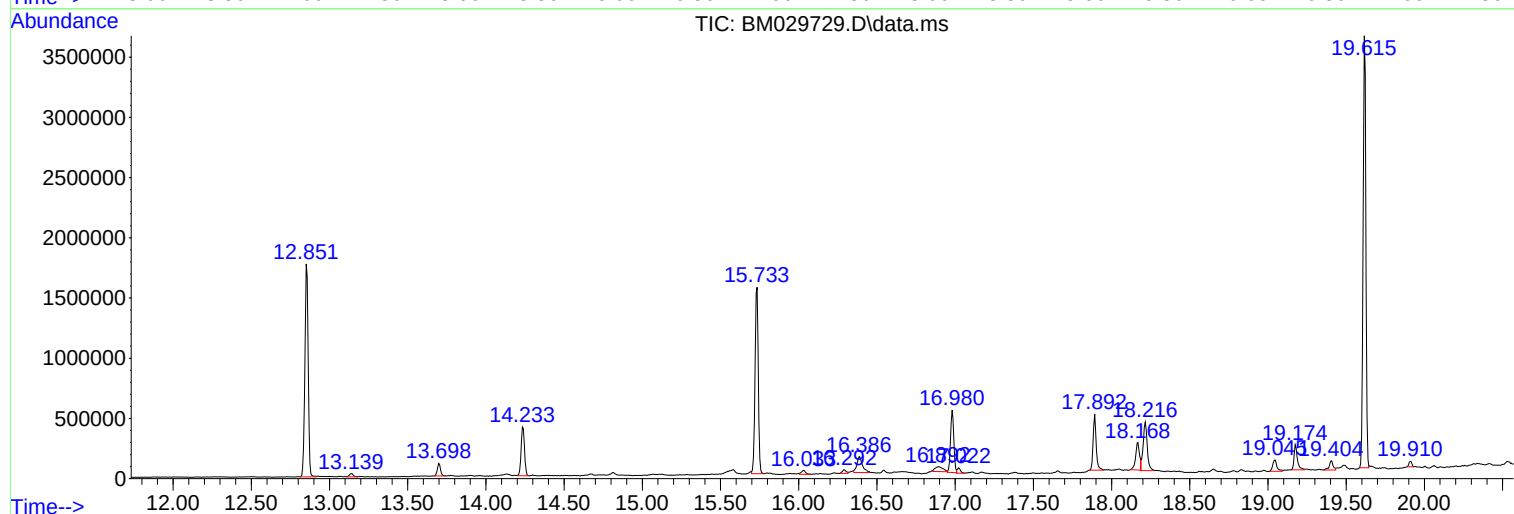
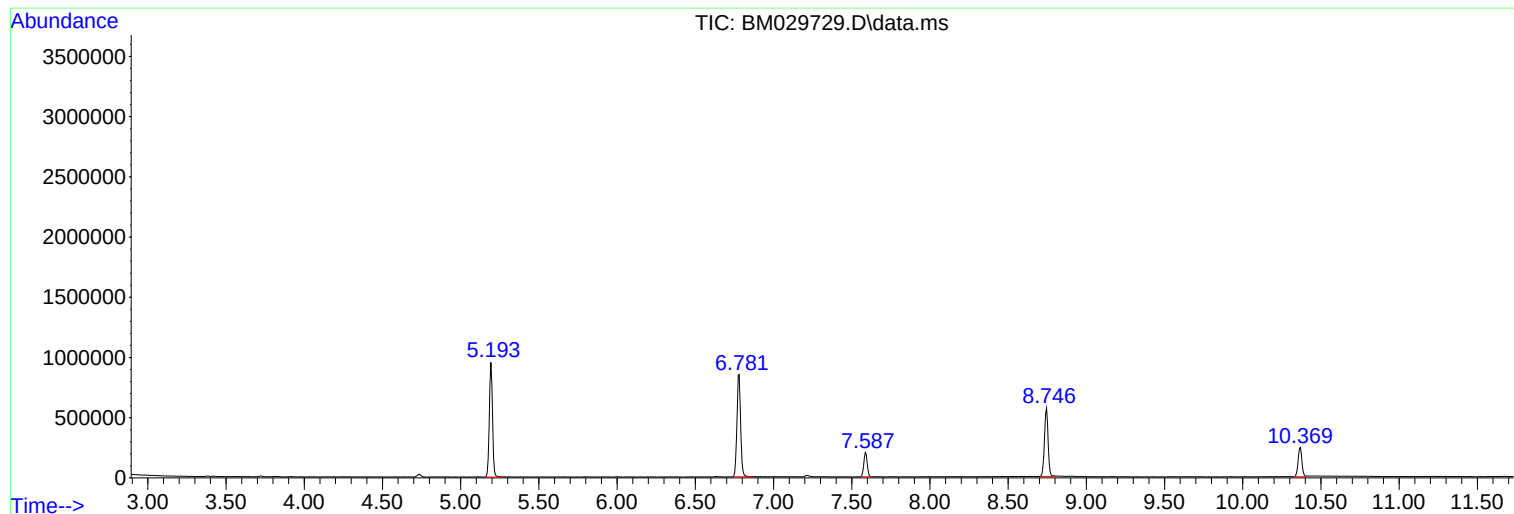
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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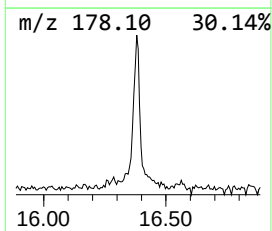
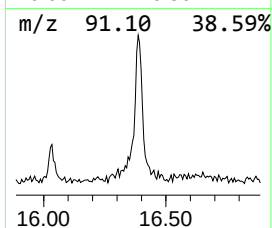
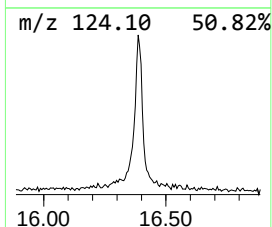
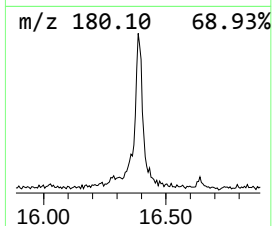
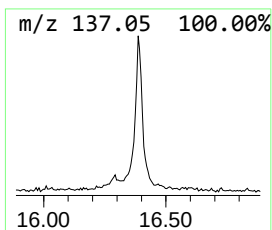
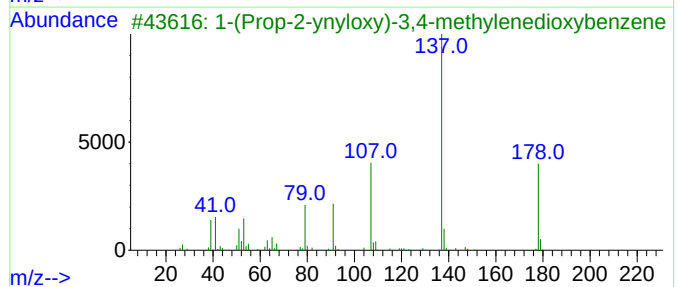
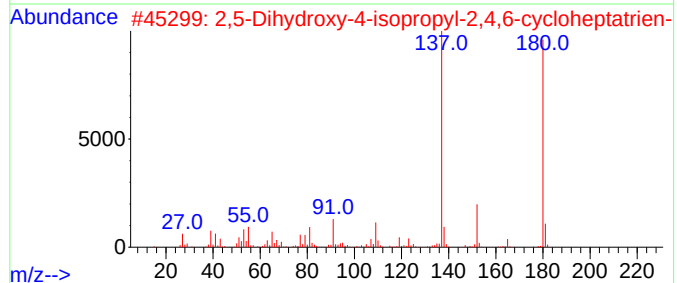
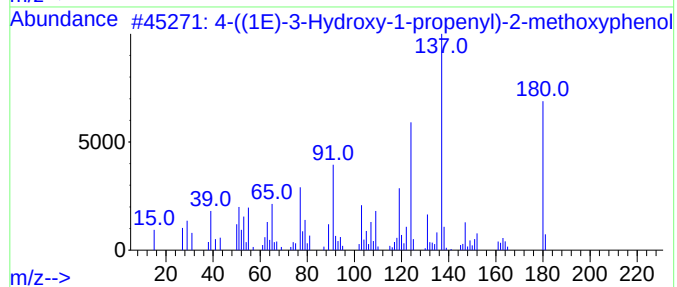
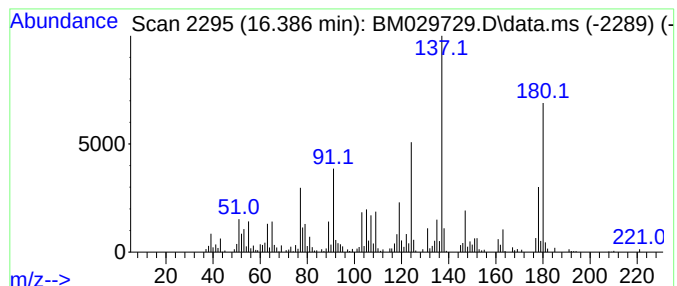
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown16.38 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.386	8.66 ng	324101	Phenanthrene-d10	16.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-((1E)-3-Hydroxy-1-propenyl)-2-...	180	C10H12O3	1000297-95-5	49		
2	2,5-Dihydroxy-4-isopropyl-2,4,6-...	180	C10H12O3	054755-56-5	38		
3	1-(Prop-2-ynyloxy)-3,4-methylene...	178	C10H10O3	019202-22-3	27		
4	6-Methylnicotinic acid	137	C7H7NO2	003222-47-7	27		
5	4-Fluorophenyl isocyanate	137	C7H4FNO	001195-45-5	22		



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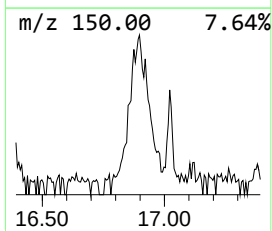
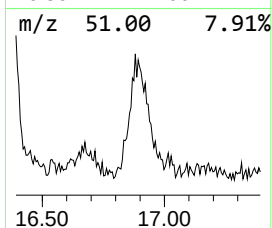
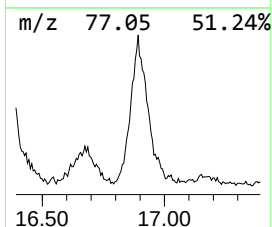
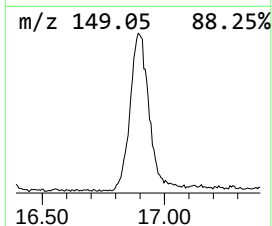
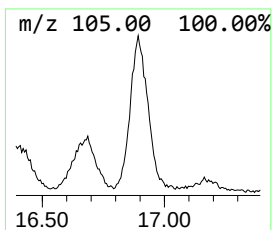
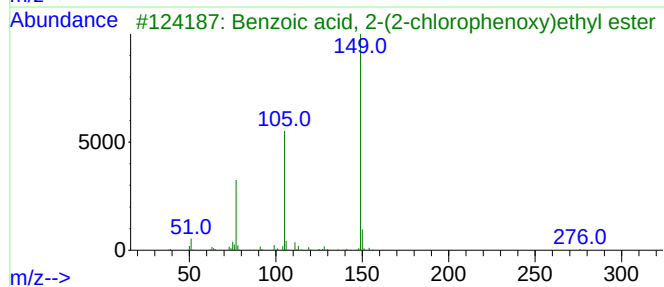
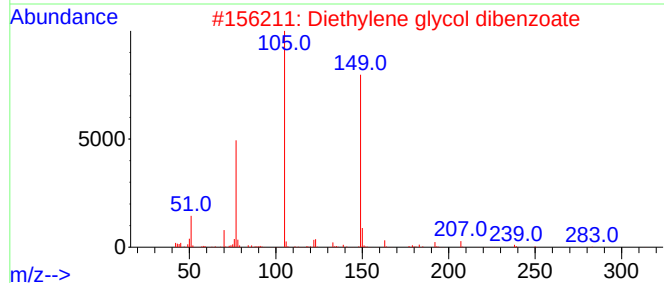
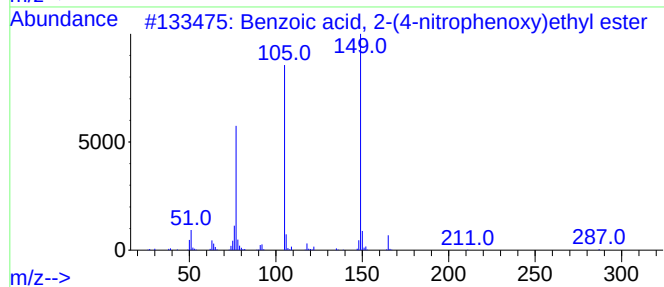
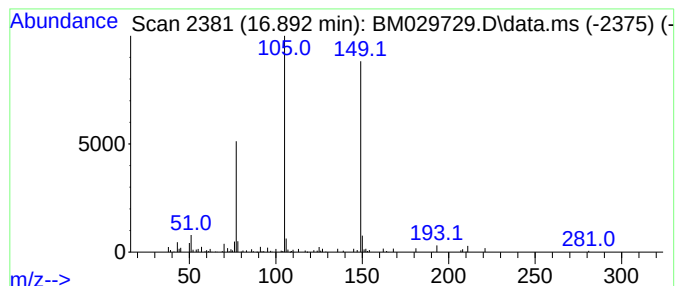
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Benzoic acid, 2-(4-nitrophe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.892	3.72 ng	139304	Phenanthrene-d10	16.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
3			Benzoic acid, 2-(2-chlorophenoxy)...	276	C15H13ClO3	1000368-25-9	59
4			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	56
5			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	53



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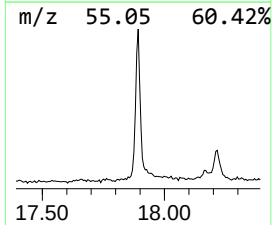
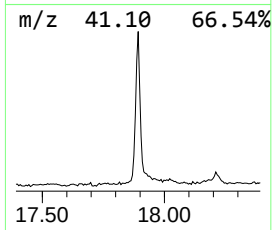
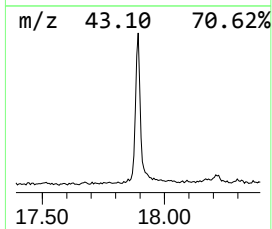
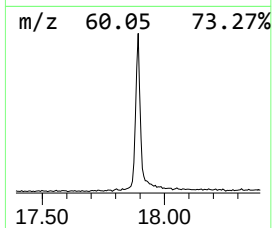
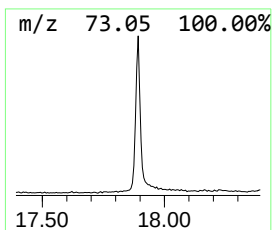
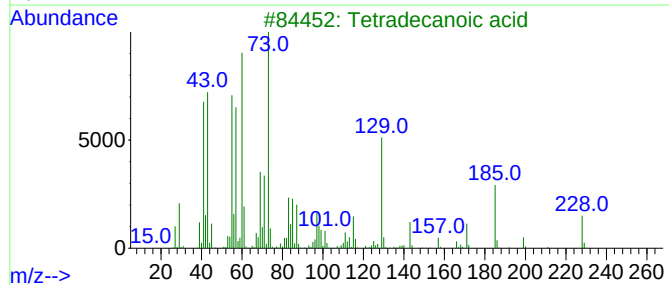
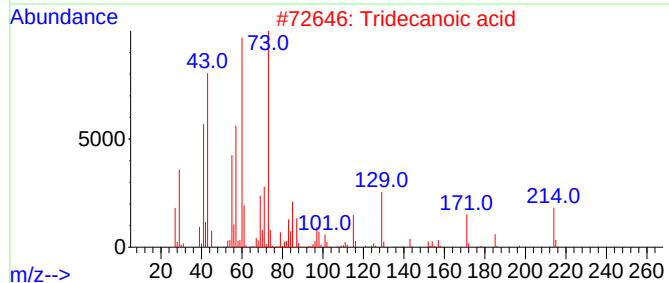
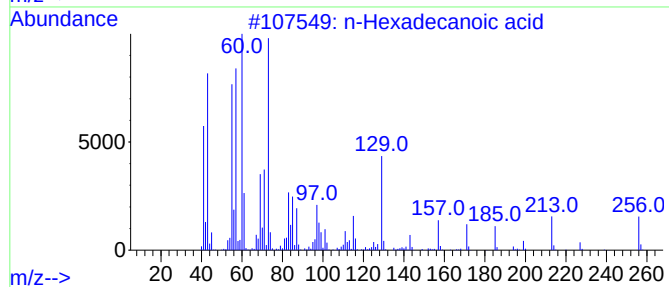
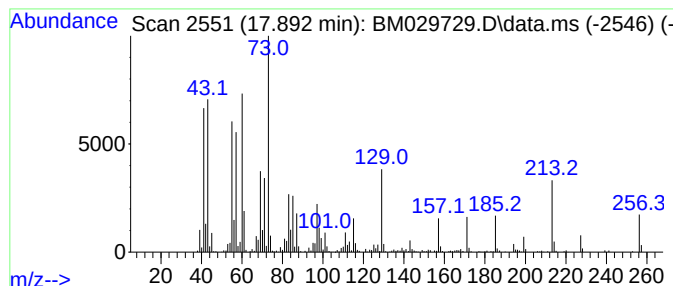
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.892	16.78 ng	627923	Phenanthrene-d10	16.980

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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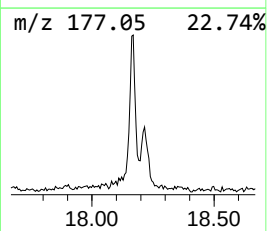
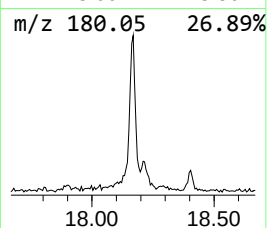
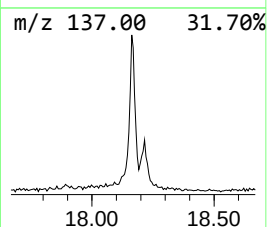
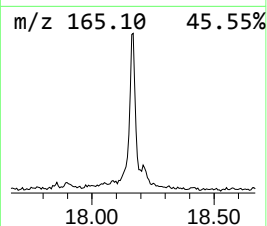
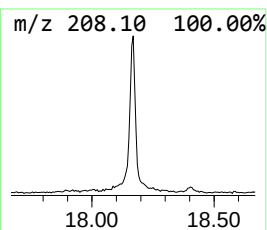
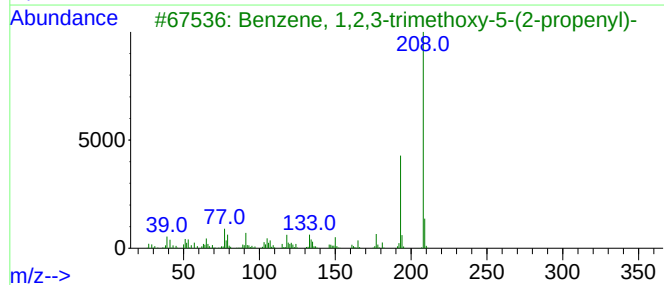
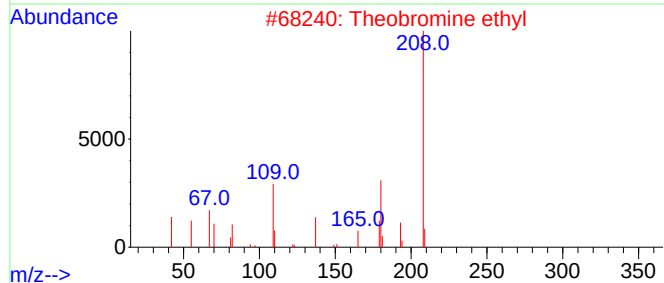
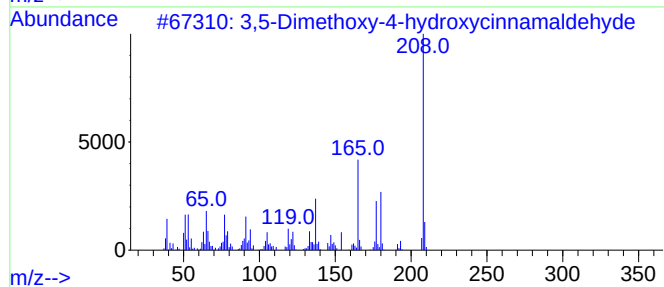
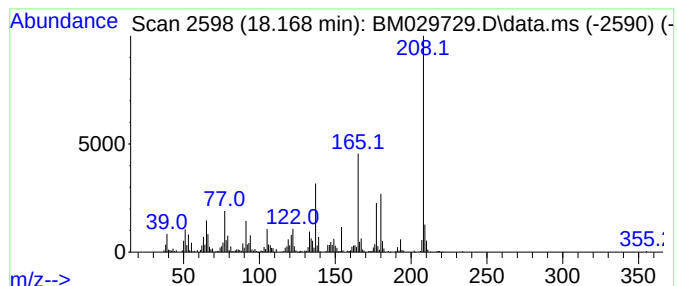
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.169	10.70 ng	400498	Phenanthrene-d10	16.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamal...	208	C11H12O4	087345-53-7	93
2	Theobromine ethyl	208	C9H12N4O2	007464-74-6	43
3	Benzene, 1,2,3-trimethoxy-5-(2-p...	208	C12H16O3	000487-11-6	38
4	2-Propenoic acid, 3-[4-(acetylox...	250	C13H14O5	002309-08-2	38
5	6,10-Dimethoxy-3,3-dimethyl-1-me...	281	C14H19NO3S	1000295-39-1	35



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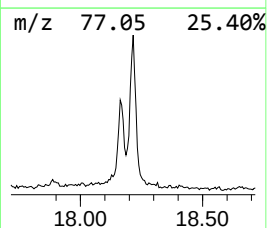
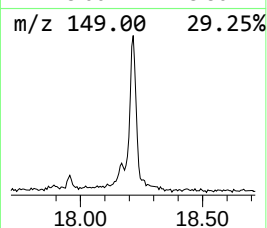
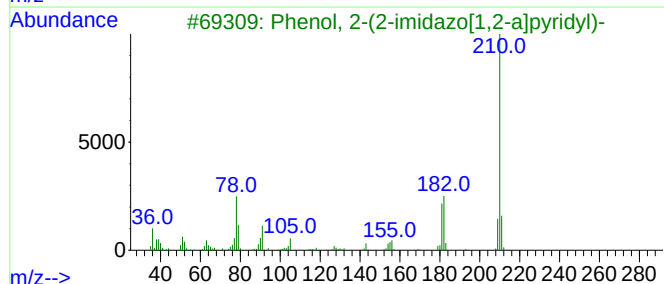
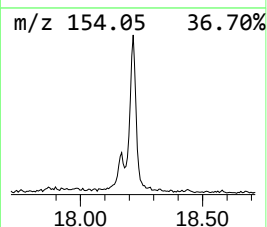
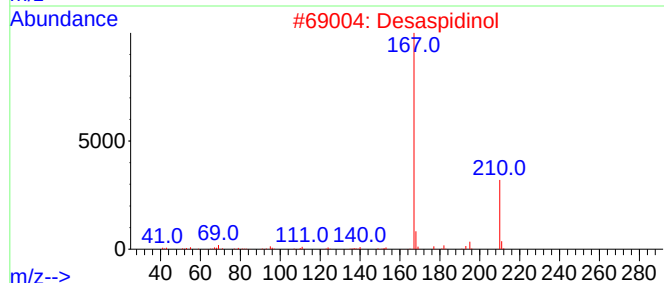
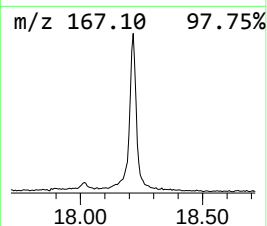
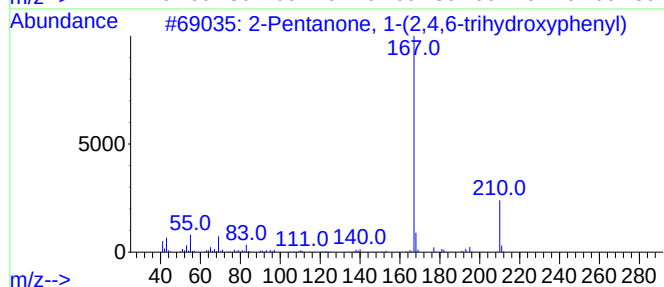
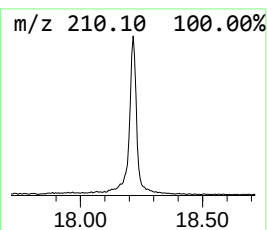
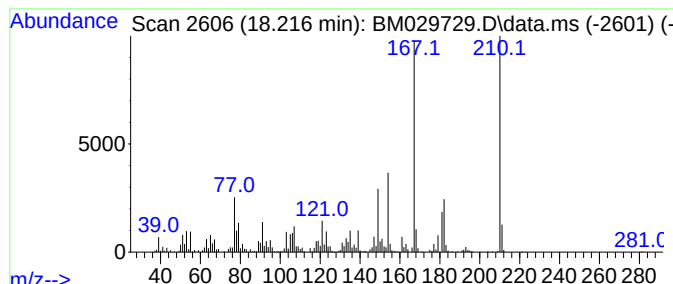
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Peak Number 5 2-Pentanone, 1-(2,4,6-trihy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	19.50 ng	729688	Phenanthrene-d10	16.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	50
2			Desaspidinol	210	C11H14O4	000437-72-9	50
3			Phenol, 2-(2-imidazo[1,2-a]pyrid...	210	C13H10N2O	057636-32-5	46
4			1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	41
5			Ethanone, 1-(2,6-dihydroxy-4-met...	182	C9H10O4	007507-89-3	38



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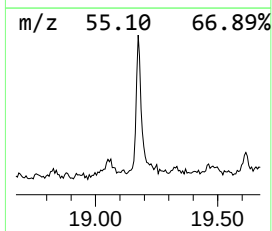
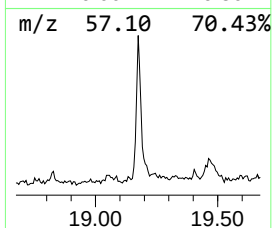
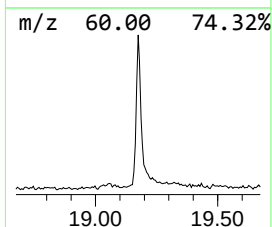
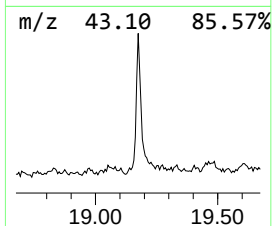
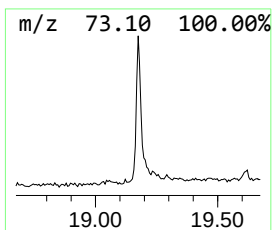
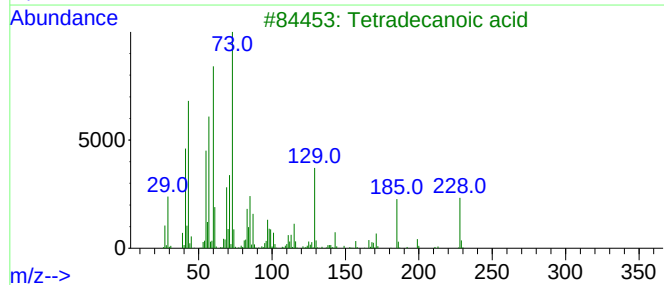
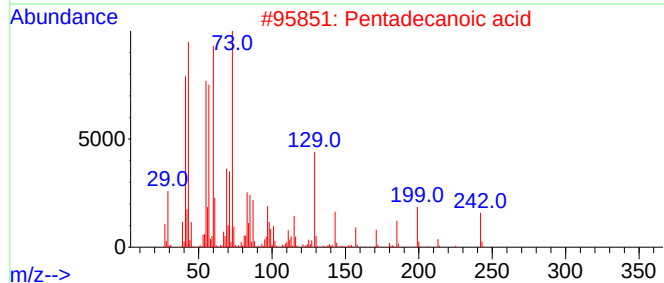
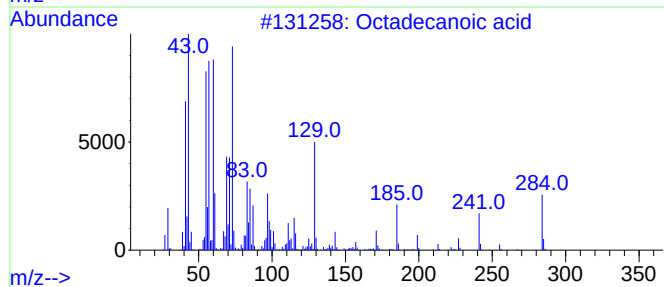
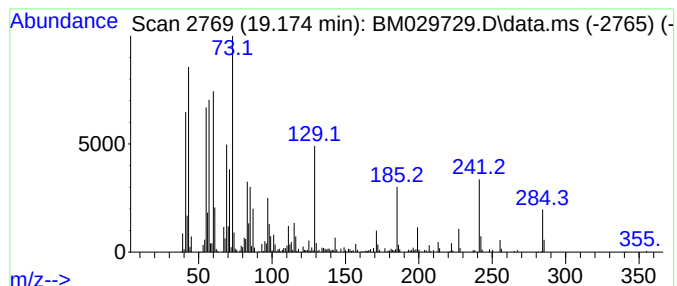
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.174	5.63 ng	301016	Chrysene-d12	21.168

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029729.D
Acq On : 30 Apr 2021 14:57
Operator : CG/JU
Sample : M2207-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-6A-5-COMP

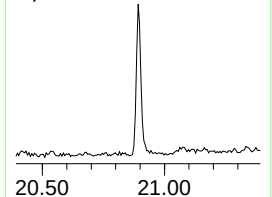
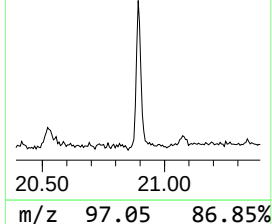
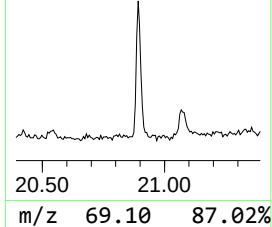
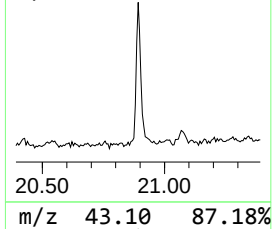
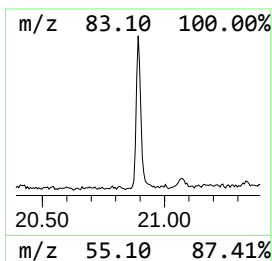
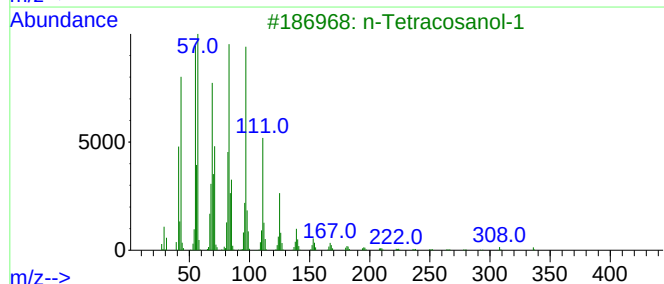
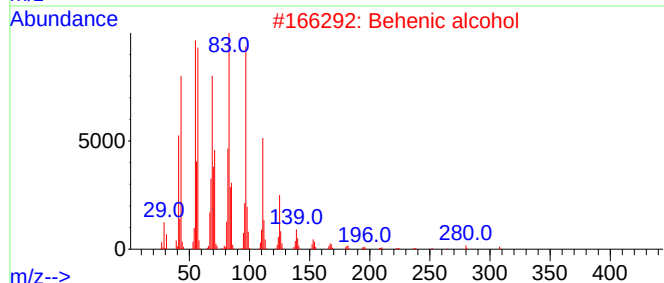
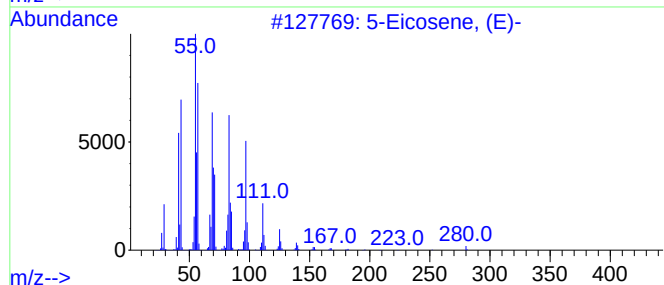
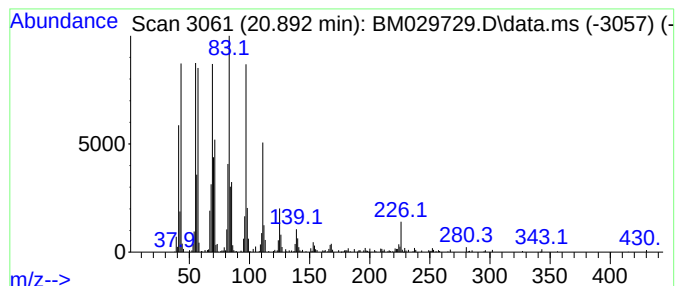
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	5.86 ng	313335	Chrysene-d12	21.168

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		Behenic alcohol	326	C22H46O	000661-19-8	95
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4		1-Heneicosanol	312	C21H44O	015594-90-8	95
5		Cetene	224	C16H32	000629-73-2	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029729.D
Acq On : 30 Apr 2021 14:57
Operator : CG/JU
Sample : M2207-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-6A-5-COMP

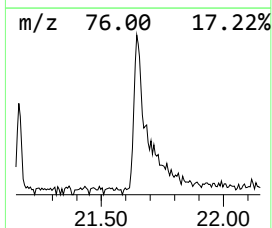
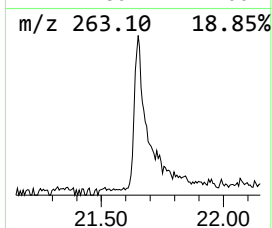
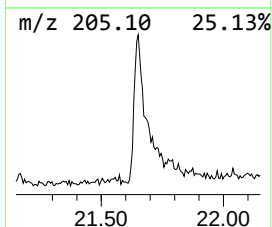
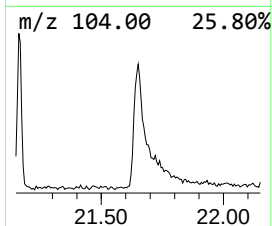
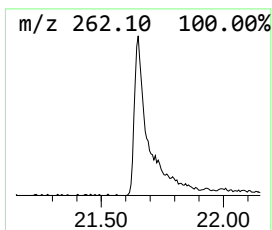
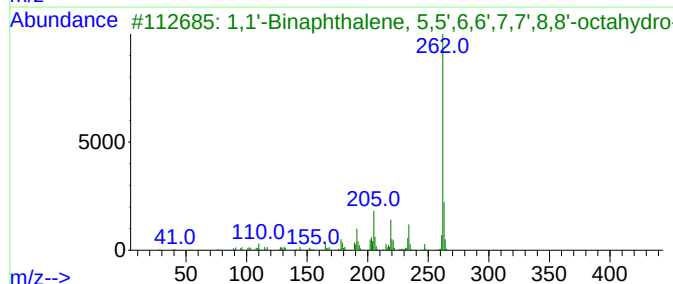
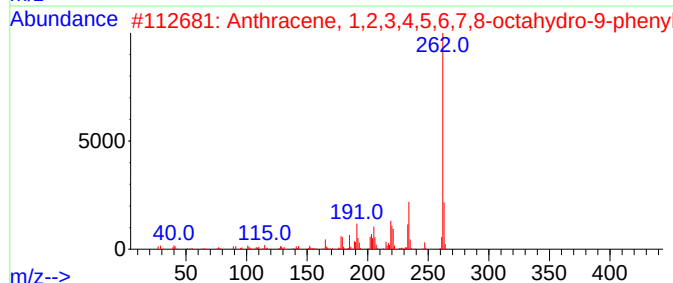
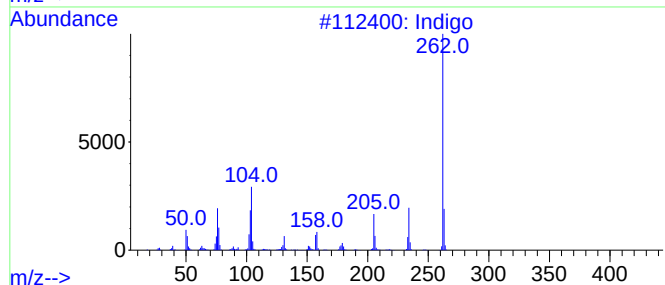
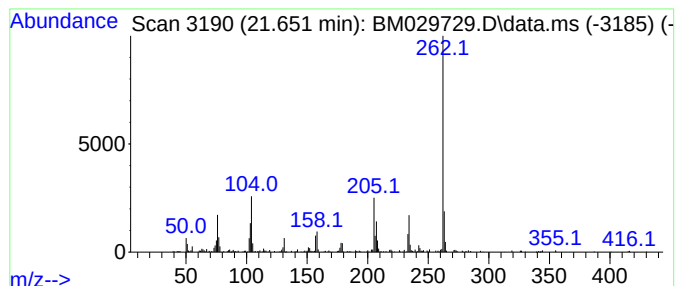
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Indigo Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.651	4.95 ng	264763	Chrysene-d12	21.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indigo	262	C16H10N2O2	000482-89-3	95
2			Anthracene, 1,2,3,4,5,6,7,8-octa...	262	C20H22	125379-29-5	58
3			1,1'-Binaphthalene, 5,5',6,6',7,...	262	C20H22	001154-14-9	53
4			1,2,3,6,7,8,9,10,11,12-Decahydro...	262	C20H22	092387-50-3	53
5			1,2,4-Oxadiazole-5-carboxylic ac...	262	C12H10N2O5	1000350-14-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029729.D
Acq On : 30 Apr 2021 14:57
Operator : CG/JU
Sample : M2207-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-6A-5-COMP

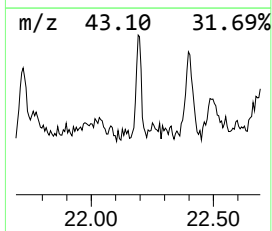
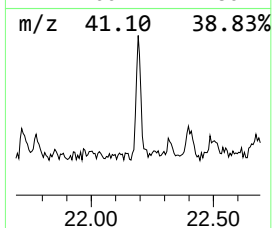
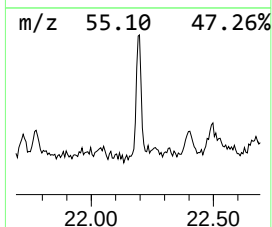
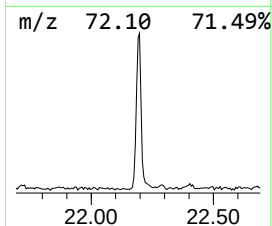
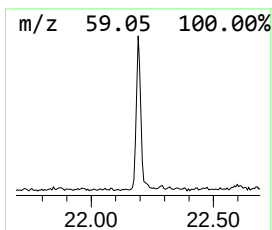
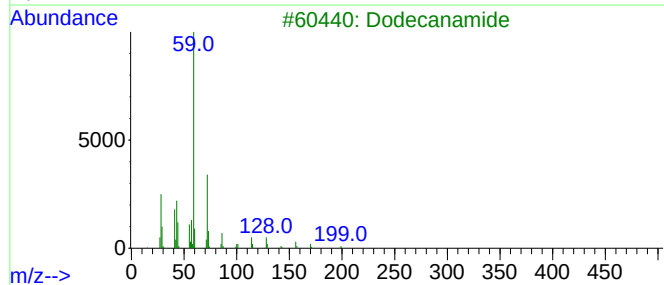
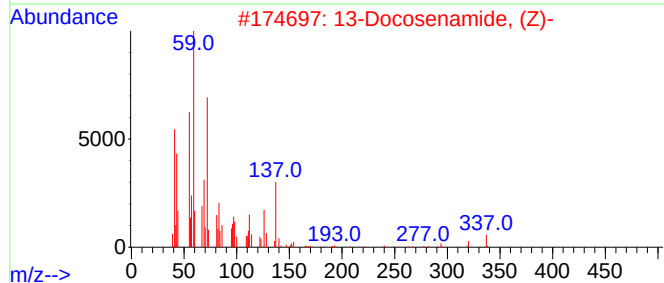
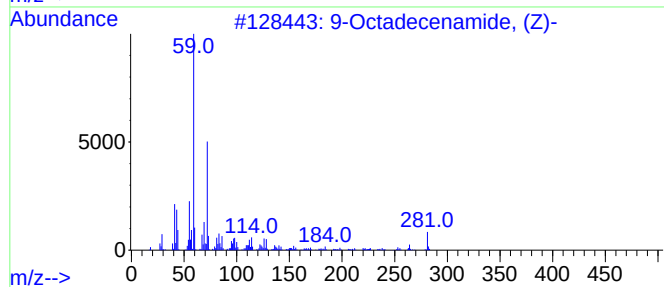
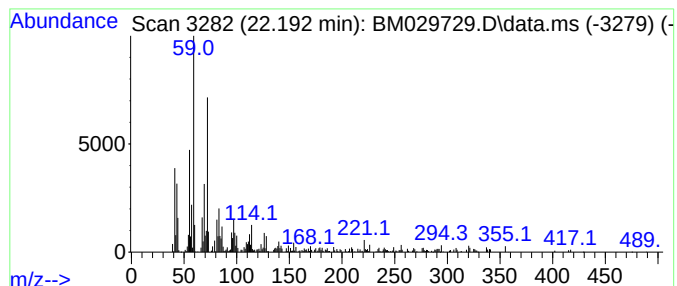
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.192	3.46 ng	184983	Chrysene-d12	21.168

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
3		Dodecanamide	199	C12H25NO	001120-16-7	58
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	58
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029729.D
Acq On : 30 Apr 2021 14:57
Operator : CG/JU
Sample : M2207-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-6A-5-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown16.38	16.386	8.7	ng	324101	4	16.980	748475	20.0
Benzoic acid, 2...	16.892	3.7	ng	139304	4	16.980	748475	20.0
n-Hexadecanoic ...	17.892	16.8	ng	627923	4	16.980	748475	20.0
3,5-Dimethoxy-4...	18.169	10.7	ng	400498	4	16.980	748475	20.0
2-Pentanone, 1-...	18.216	19.5	ng	729688	4	16.980	748475	20.0
Octadecanoic acid	19.174	5.6	ng	301016	5	21.168	1069380	20.0
5-Eicosene, (E)-	20.892	5.9	ng	313335	5	21.168	1069380	20.0
Indigo	21.651	5.0	ng	264763	5	21.168	1069380	20.0
9-Octadecenamid...	22.192	3.5	ng	184983	5	21.168	1069380	20.0