

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121021\
 Data File : BM033399.D
 Acq On : 10 Dec 2021 18:01
 Operator : CG/JU
 Sample : M4989-15
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P6-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-BM120821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.031	300	305	313	rVB	355988	529721	14.59%	2.208%
2	5.490	377	383	389	rBV	1972284	2865707	78.95%	11.943%
3	5.549	389	393	402	rVB2	86658	189137	5.21%	0.788%
4	5.919	452	456	462	rVB2	40369	64903	1.79%	0.270%
5	6.101	483	487	492	rVB	37474	57155	1.57%	0.238%
6	7.078	646	653	666	rBV	1854958	3060266	84.31%	12.754%
7	7.901	787	793	801	rVB	320069	519748	14.32%	2.166%
8	9.066	984	991	1001	rBV	1187030	1981083	54.58%	8.256%
9	10.478	1226	1231	1244	rBV3	25864	50574	1.39%	0.211%
10	10.695	1261	1268	1277	rBV	386439	693527	19.11%	2.890%
11	13.154	1676	1686	1697	rBV	2370602	3581054	98.66%	14.924%
12	13.342	1713	1718	1721	rBV3	35964	50722	1.40%	0.211%
13	14.166	1853	1858	1865	rBV6	24765	46456	1.28%	0.194%
14	14.413	1891	1900	1905	rBV3	36332	81768	2.25%	0.341%
15	14.530	1913	1920	1932	rVB	518883	811558	22.36%	3.382%
16	15.930	2153	2158	2164	rBV	105633	138965	3.83%	0.579%
17	16.013	2166	2172	2189	rVV	1427040	2181427	60.10%	9.091%
18	17.265	2378	2385	2391	rBV	547024	831427	22.91%	3.465%
19	17.383	2401	2405	2411	rVB5	69473	95840	2.64%	0.399%
20	17.548	2429	2433	2440	rVB	29060	46055	1.27%	0.192%
21	17.918	2492	2496	2501	rVB5	50217	76592	2.11%	0.319%
22	18.148	2531	2535	2540	rBV3	60222	86436	2.38%	0.360%
23	18.224	2545	2548	2553	rVV	53069	64813	1.79%	0.270%
24	18.442	2581	2585	2589	rBV2	31418	44814	1.23%	0.187%
25	18.995	2676	2679	2684	rBV3	28730	38071	1.05%	0.159%
26	19.312	2729	2733	2739	rVB6	30215	61825	1.70%	0.258%
27	19.877	2824	2829	2838	rVB	2804858	3629629	100.00%	15.127%
28	20.630	2953	2957	2960	rBV	70632	79042	2.18%	0.329%
29	21.124	3037	3041	3047	rBV	226315	293487	8.09%	1.223%
30	21.330	3073	3076	3081	rVB	122848	140722	3.88%	0.586%
31	21.430	3088	3093	3100	rBV	599856	778315	21.44%	3.244%
32	22.283	3235	3238	3244	rVB2	81035	102166	2.81%	0.426%
33	23.747	3481	3487	3497	rVB	365000	721601	19.88%	3.007%

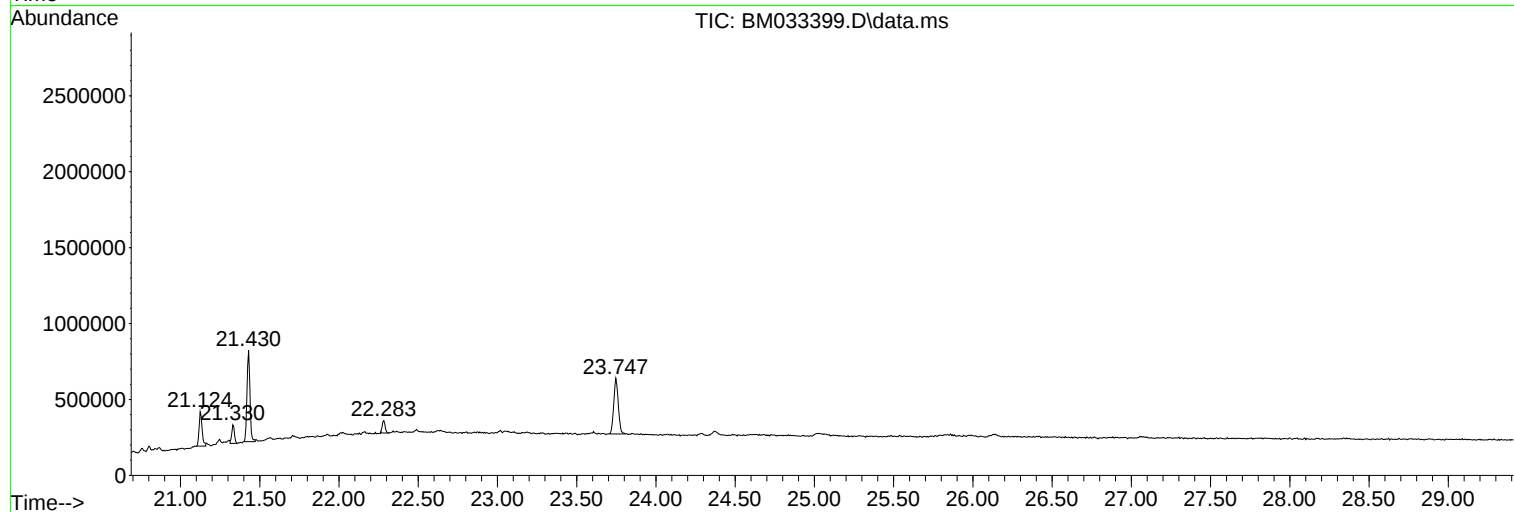
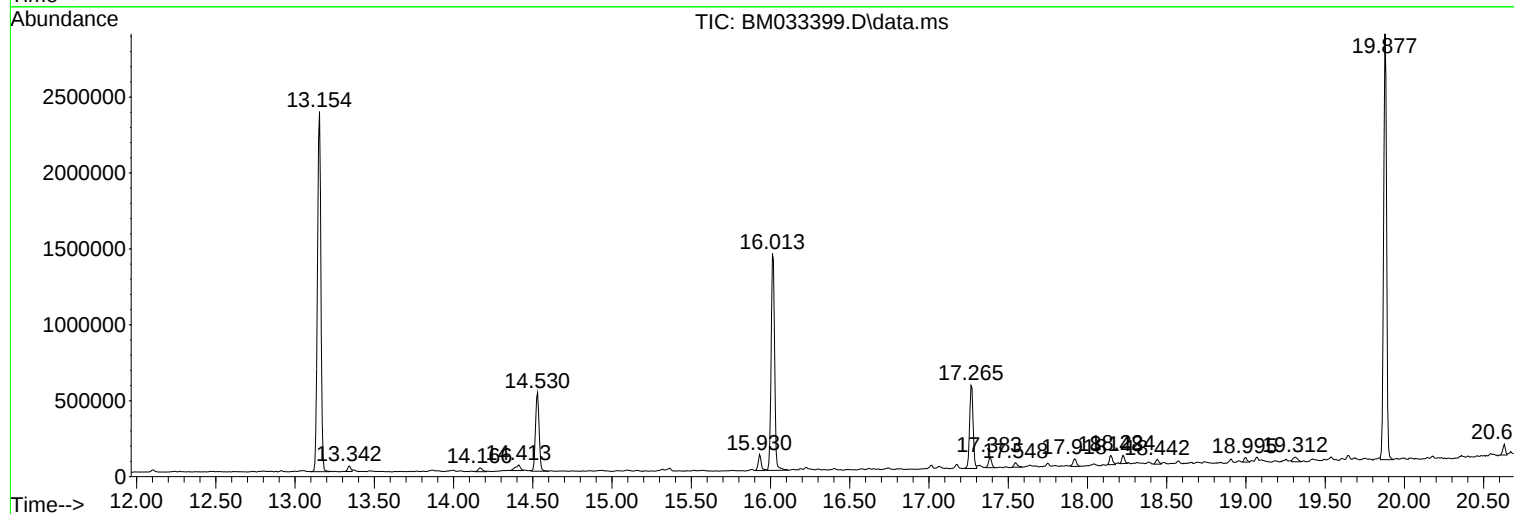
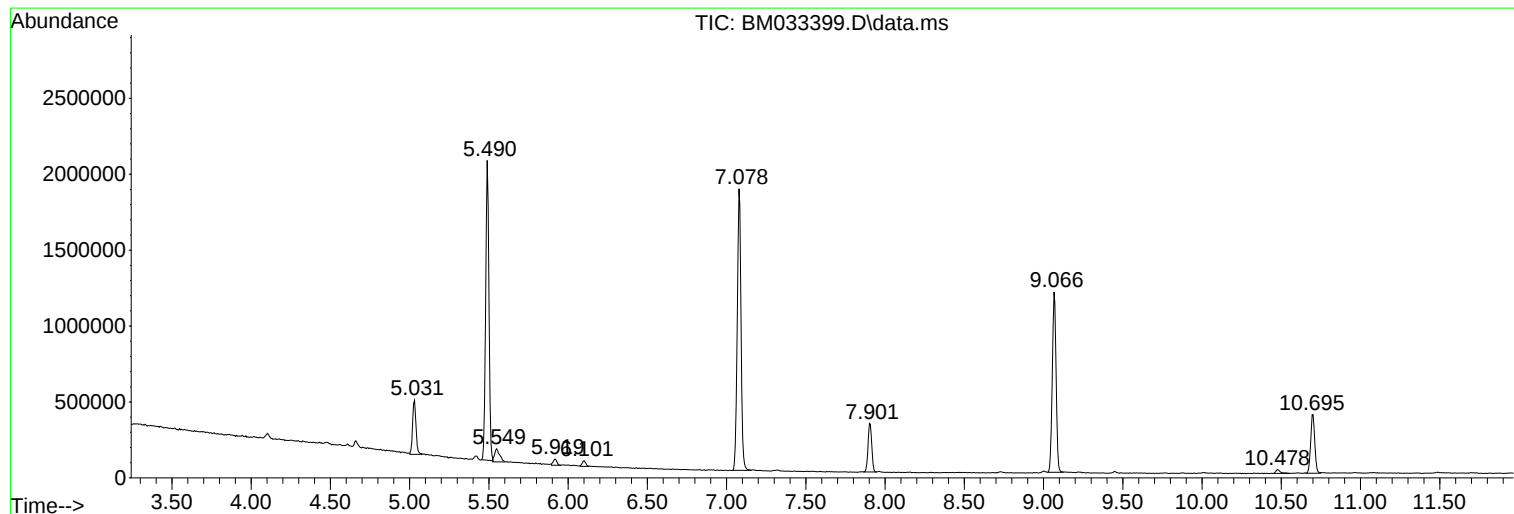
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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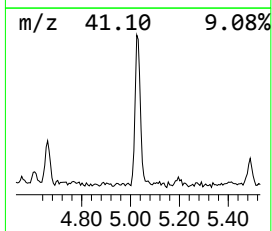
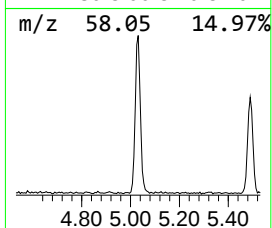
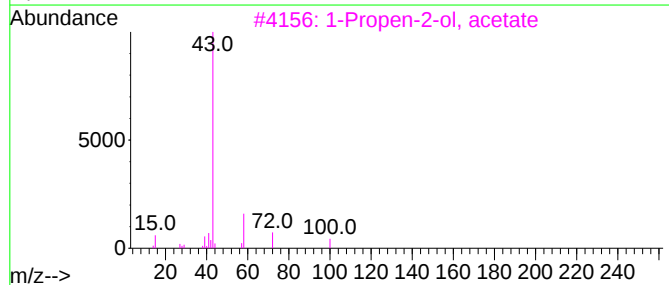
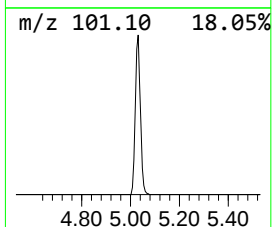
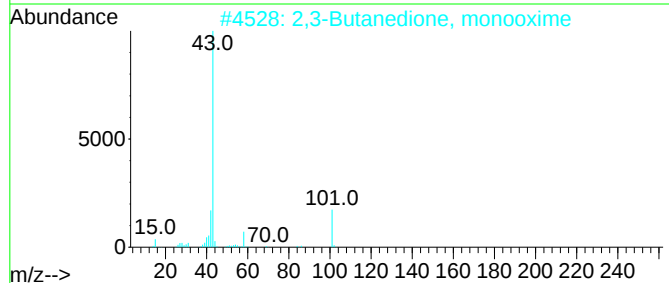
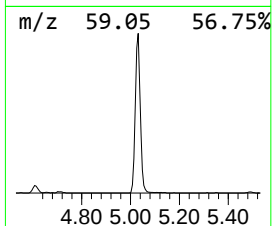
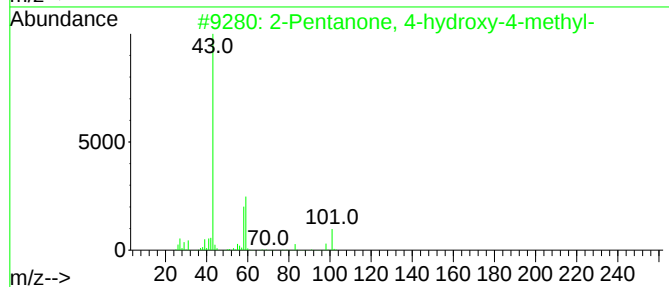
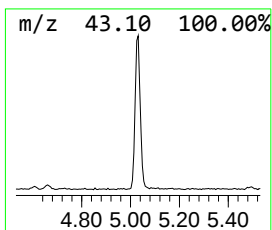
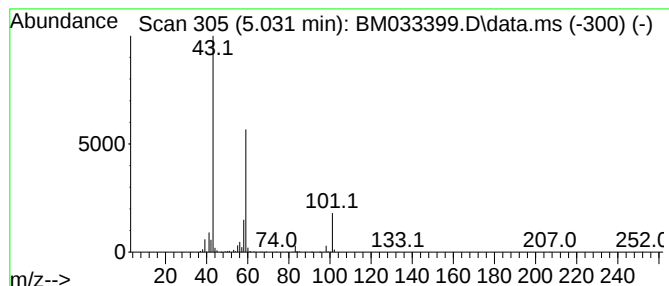
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.031	20.38 ng	529721	1,4-Dichlorobenzene-d4	7.901

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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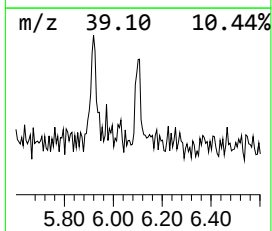
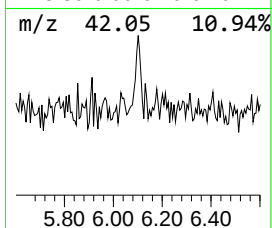
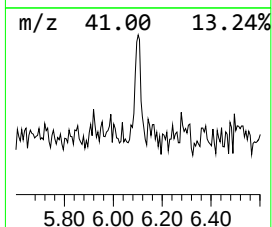
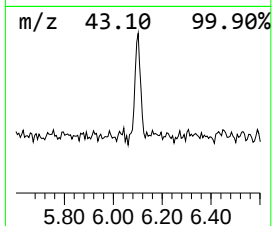
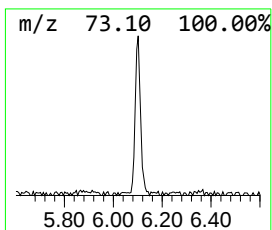
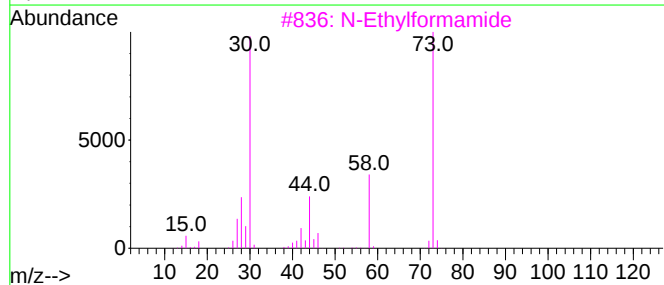
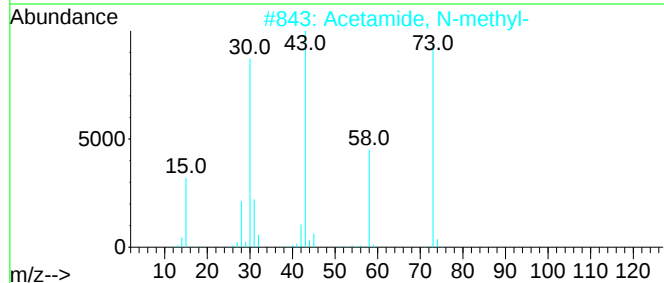
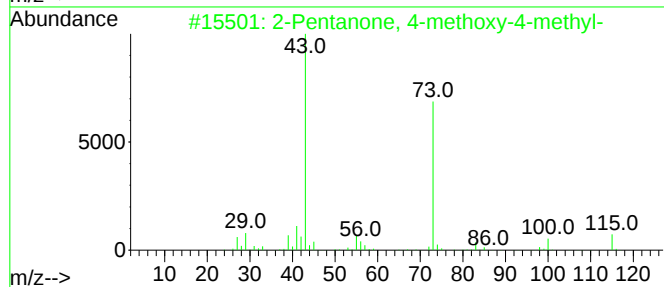
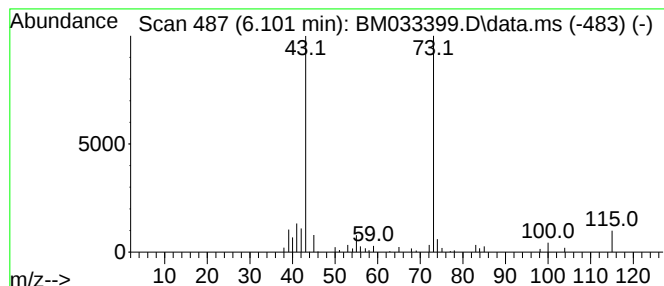
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.101	2.20 ng	57155	1,4-Dichlorobenzene-d4	7.901

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	40
3			N-Ethylformamide	73	C3H7NO	000627-45-2	32
4			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	12



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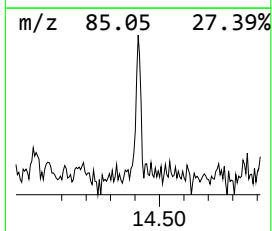
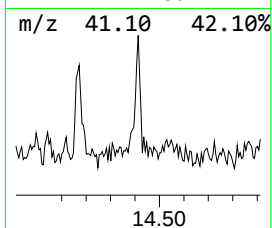
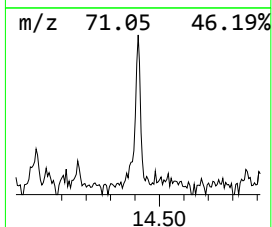
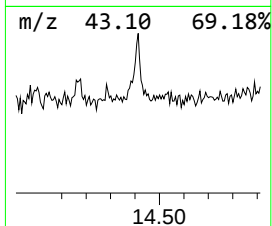
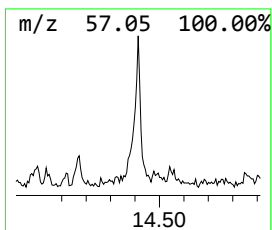
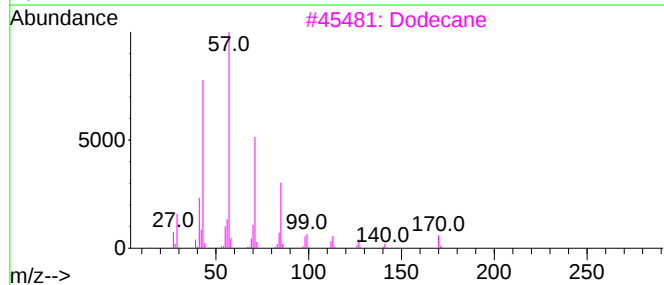
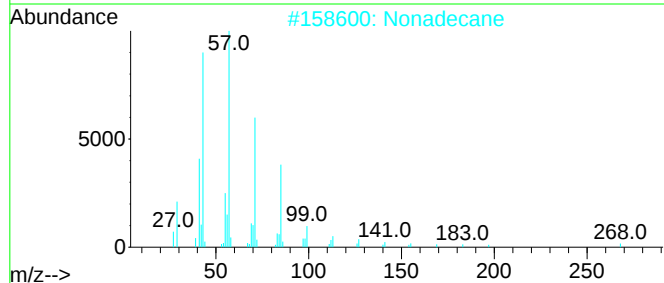
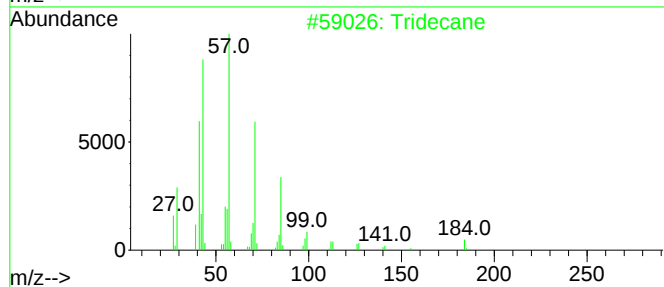
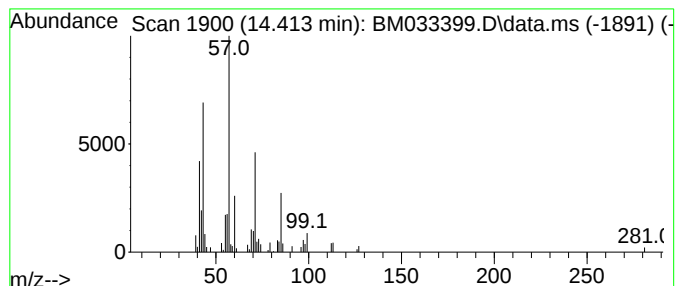
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.413	2.02 ng	81768	Acenaphthene-d10	14.530

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	64
2			Nonadecane	268	C19H40	000629-92-5	58
3			Dodecane	170	C12H26	000112-40-3	58
4			Hexadecane	226	C16H34	000544-76-3	58
5			Tetradecane	198	C14H30	000629-59-4	58



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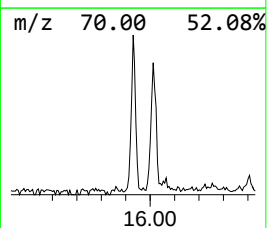
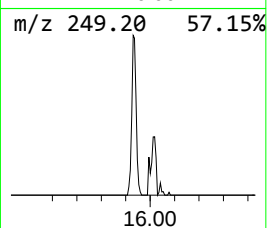
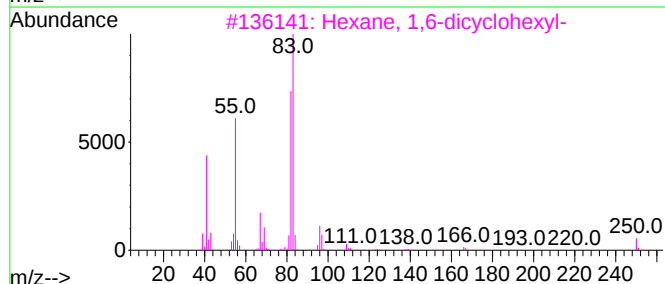
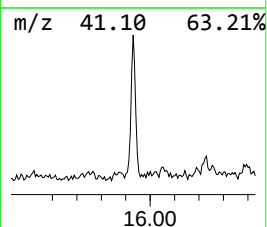
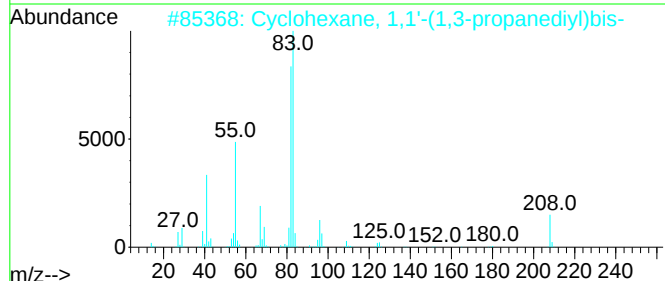
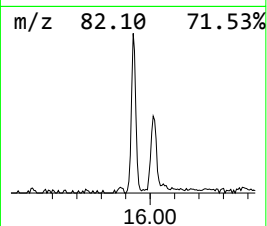
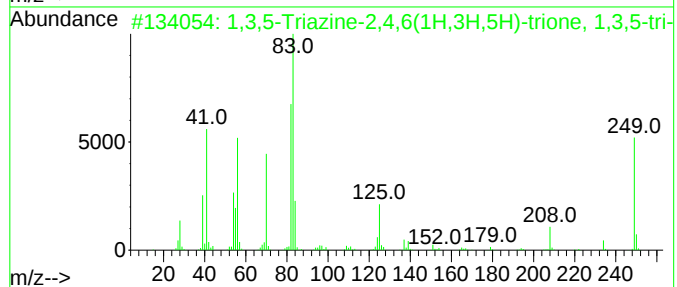
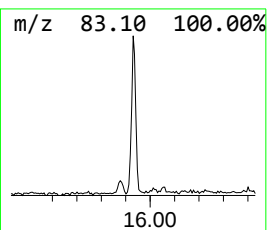
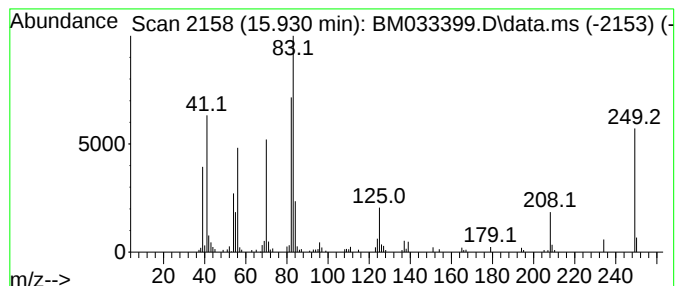
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Peak Number 6 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.930	3.34 ng	138965	Phenanthrene-d10	17.265

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	99
2		Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	35
3		Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	25
4		Imidazole, 2-acetamido-	125	C5H7N3O	052737-49-2	17
5		1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	16



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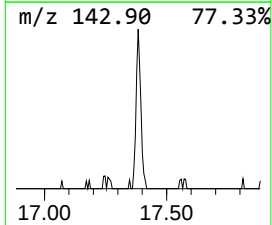
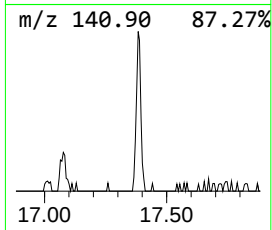
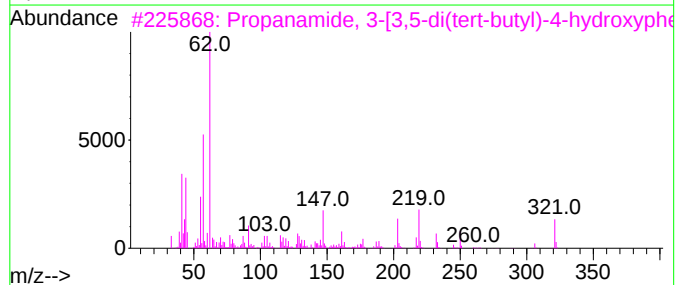
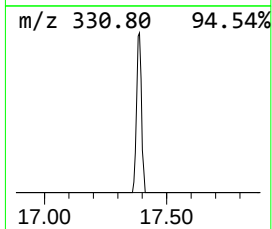
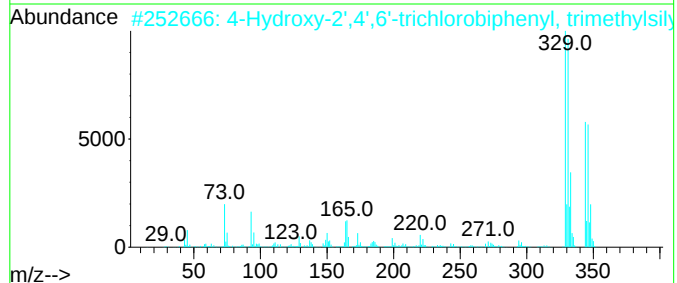
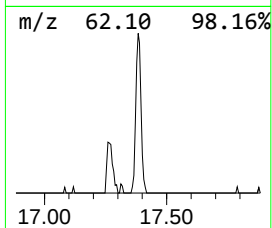
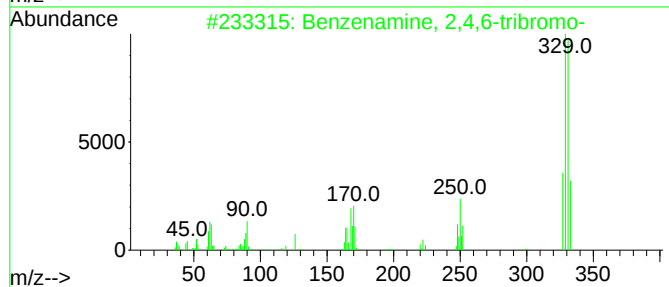
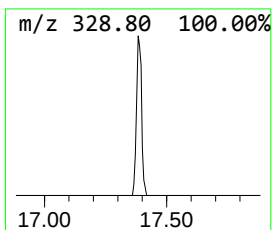
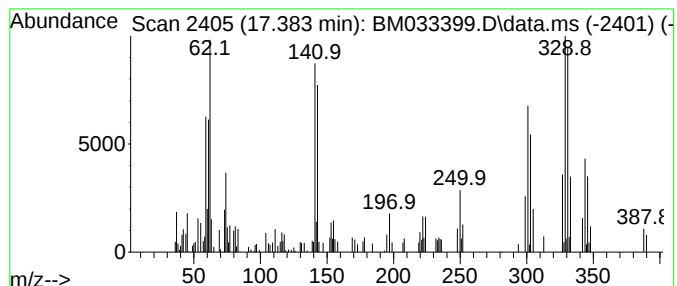
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Peak Number 7 unknown17.383 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.383	2.31 ng	95840	Phenanthrene-d10	17.265

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	25
2			4-Hydroxy-2',4',6'-trichlorobiph...	344	C15H15Cl3OSi	1000447-71-9	18
3			Propanamide, 3-[3,5-di(tert-buty...	321	C19H31NO3	1000294-01-1	12
4			Tellurium, bis[(.eta.-5-cyclopen...	612	C22H40Ni2P2Te	1000161-69-8	12
5			Triethylphosphine	118	C6H15P	000554-70-1	12



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Misc :
ALS Vial : 10 Sample Multiplier: 1

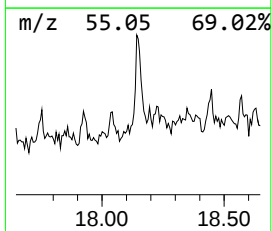
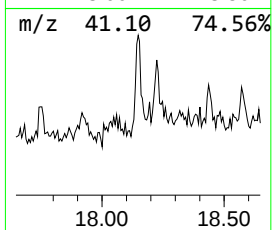
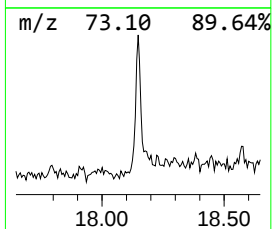
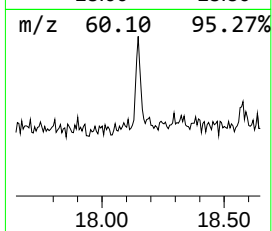
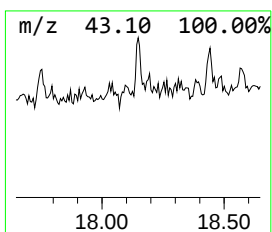
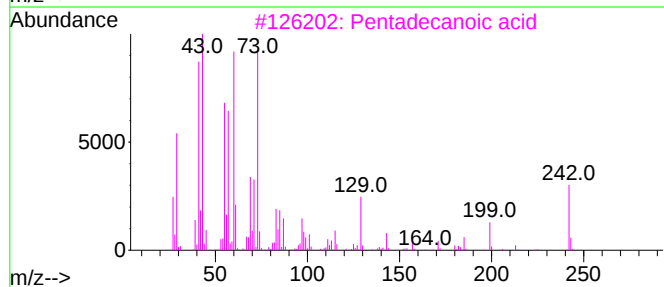
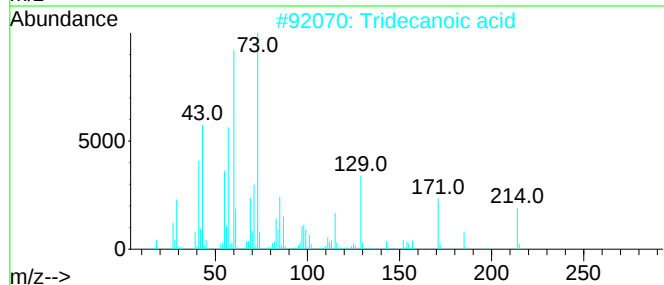
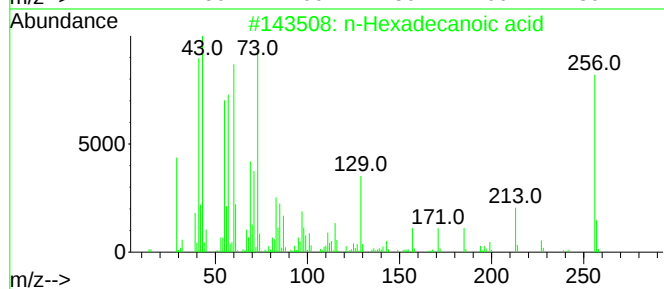
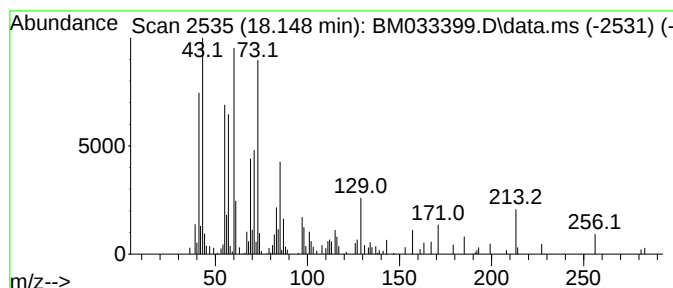
Instrument :
BNA_M
ClientSampleId :
P6-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.148	2.08 ng	86436	Phenanthrene-d10	17.265	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121021\
Data File : BM033399.D
Acq On : 10 Dec 2021 18:01
Operator : CG/JU
Sample : M4989-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P6-COMP

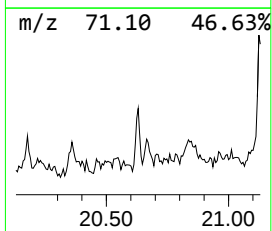
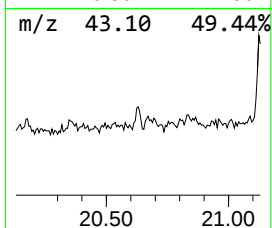
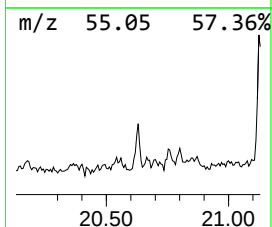
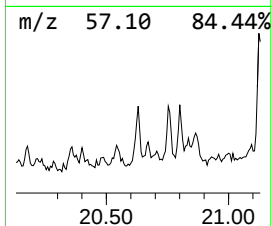
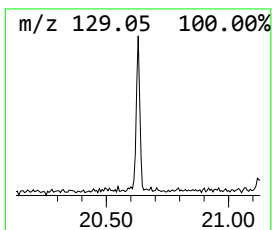
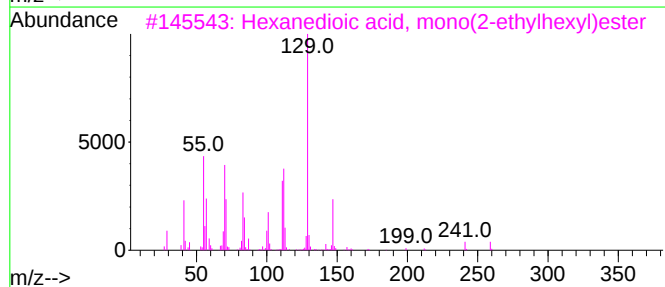
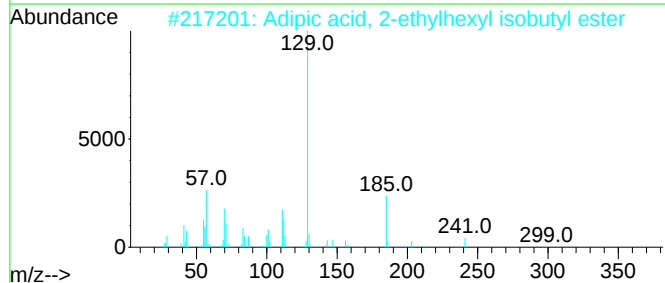
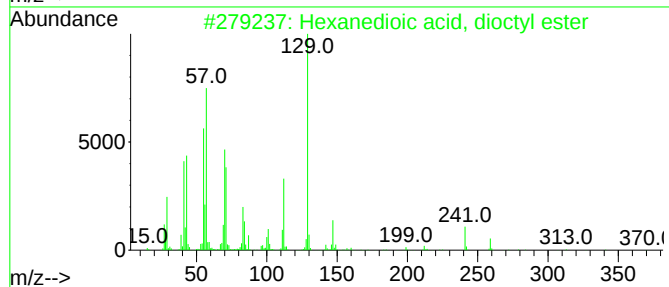
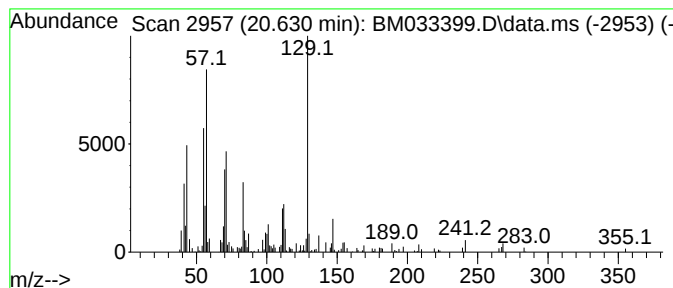
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexanedioic acid, dioctyl e... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.630	2.03 ng	79042	Chrysene-d12	21.430

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	53
2			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	47
3			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	46
4			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	46
5			Adipic acid, 2-octyl undecyl ester	412	C25H48O4	1000324-45-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121021\
Data File : BM033399.D
Acq On : 10 Dec 2021 18:01
Operator : CG/JU
Sample : M4989-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

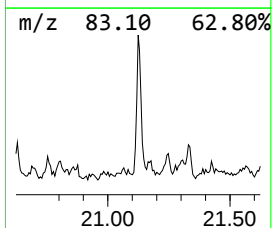
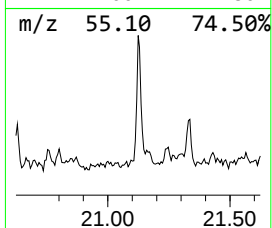
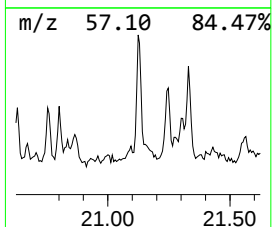
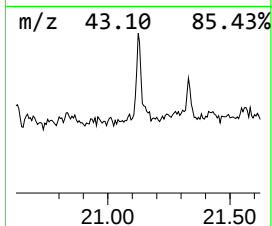
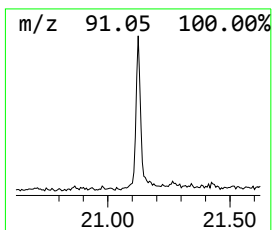
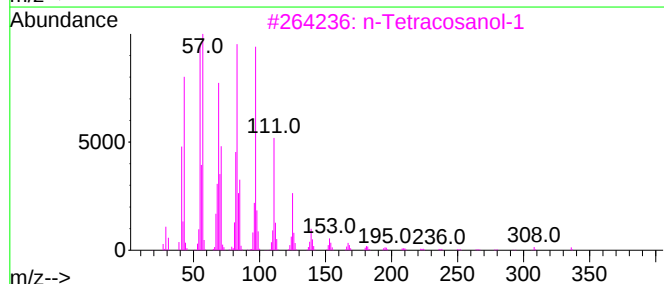
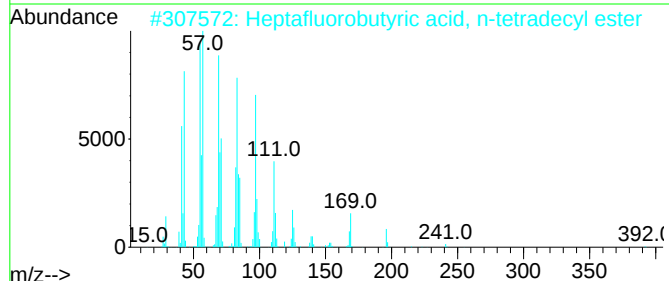
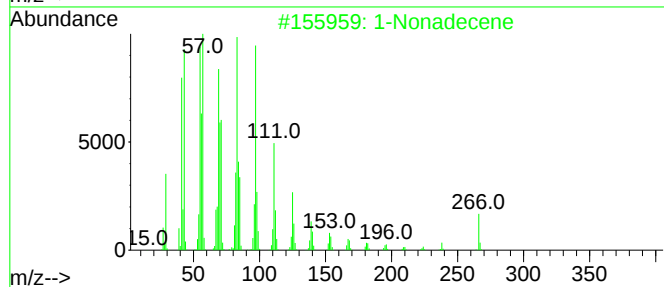
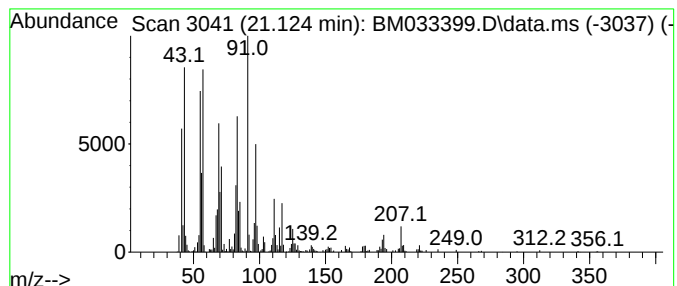
Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Nonadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.124	7.54 ng	293487	Chrysene-d12	21.430	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	93
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121021\
Data File : BM033399.D
Acq On : 10 Dec 2021 18:01
Operator : CG/JU
Sample : M4989-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P6-COMP

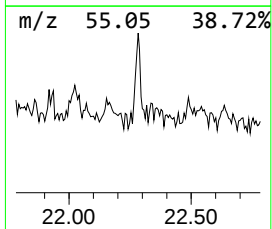
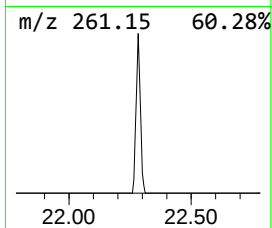
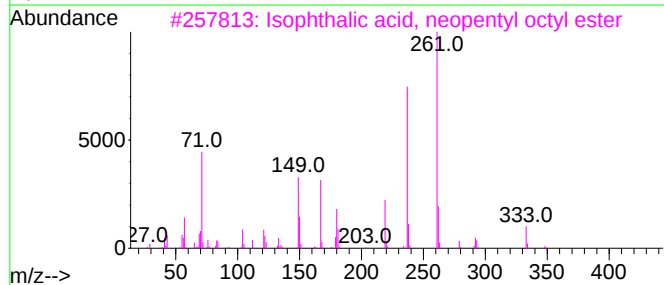
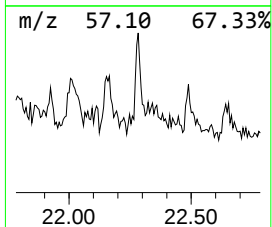
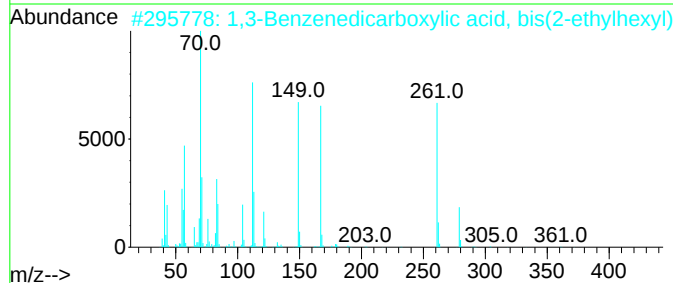
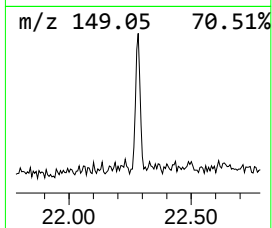
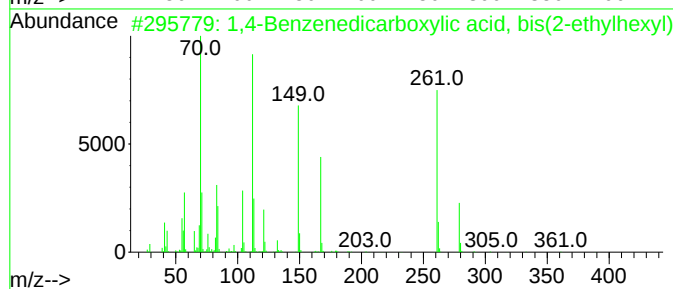
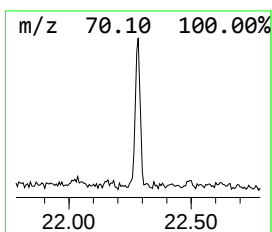
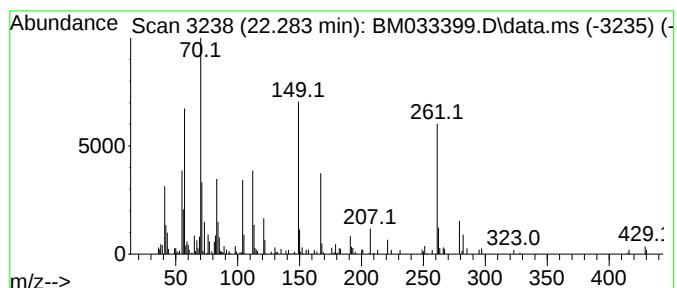
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.283	2.63 ng	102166	Chrysene-d12	21.430

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
3			Isophthalic acid, neopentyl octy...	348	C21H32O4	1000343-86-6	22
4			Isophthalic acid, octyl 1-propyl...	376	C23H36O4	1000356-40-3	22
5			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121021\
Data File : BM033399.D
Acq On : 10 Dec 2021 18:01
Operator : CG/JU
Sample : M4989-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P6-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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-...	5.031	20.4	ng	529721	1	7.901	519748	20.0
2-Pentanone, 4-...	6.101	2.2	ng	57155	1	7.901	519748	20.0
Tridecane	14.413	2.0	ng	81768	3	14.530	811558	20.0
1,3,5-Triazine-...	15.930	3.3	ng	138965	4	17.265	831427	20.0
unknown17.383	17.383	2.3	ng	95840	4	17.265	831427	20.0
n-Hexadecanoic ...	18.148	2.1	ng	86436	4	17.265	831427	20.0
Hexanedioic aci...	20.630	2.0	ng	79042	5	21.430	778315	20.0
1-Nonadecene	21.124	7.5	ng	293487	5	21.430	778315	20.0
1,4-Benzenedica...	22.283	2.6	ng	102166	5	21.430	778315	20.0