

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
 Data File : BP008281.D
 Acq On : 08 Dec 2021 15:34
 Operator : CG/JU
 Sample : M4953-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A377

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_P\Methods\8270E-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008281.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	320	326	333	rVB	79713	114581	2.36%	0.518%
2	5.369	399	405	423	rVB	724093	1075551	22.18%	4.862%
3	6.963	662	676	691	rBV	371665	701500	14.47%	3.171%
4	7.775	805	814	821	rBV	321199	523411	10.80%	2.366%
5	8.940	997	1012	1024	rBV	1173238	2012786	41.51%	9.098%
6	10.381	1249	1257	1273	rBV	43528	107391	2.21%	0.485%
7	10.569	1282	1289	1299	rBV	393321	675285	13.93%	3.053%
8	12.281	1572	1580	1589	rBV2	25002	78054	1.61%	0.353%
9	13.045	1702	1710	1720	rBV	2950124	4328671	89.28%	19.567%
10	14.093	1882	1888	1899	rBV2	37496	76133	1.57%	0.344%
11	14.428	1937	1945	1952	rBV	582145	893963	18.44%	4.041%
12	15.257	2078	2086	2090	rBV2	52108	119883	2.47%	0.542%
13	15.928	2193	2200	2208	rBV	1540853	2281081	47.05%	10.311%
14	17.116	2398	2402	2407	rVB	57354	72003	1.49%	0.325%
15	17.192	2408	2415	2424	rBV	640074	958701	19.77%	4.334%
16	17.492	2460	2466	2475	rBV3	23126	56614	1.17%	0.256%
17	18.092	2564	2568	2574	rBV	80682	116570	2.40%	0.527%
18	18.504	2634	2638	2643	rVB2	47234	55092	1.14%	0.249%
19	19.333	2775	2779	2787	rBV6	27630	49712	1.03%	0.225%
20	19.763	2847	2852	2861	rBV	3768817	4848525	100.00%	21.917%
21	20.445	2964	2968	2974	rBV	93728	117498	2.42%	0.531%
22	20.516	2977	2980	2983	rVB	46037	49015	1.01%	0.222%
23	20.974	3054	3058	3061	rBV	44828	67167	1.39%	0.304%
24	21.016	3061	3065	3071	rVV2	225299	346267	7.14%	1.565%
25	21.080	3072	3076	3082	rVV	83733	116285	2.40%	0.526%
26	21.210	3095	3098	3102	rBV	107191	115455	2.38%	0.522%
27	21.298	3108	3113	3117	rBV	731630	1002824	20.68%	4.533%
28	22.545	3322	3325	3329	rVB	92315	115326	2.38%	0.521%
29	23.692	3514	3520	3529	rVB2	498827	1046973	21.59%	4.733%

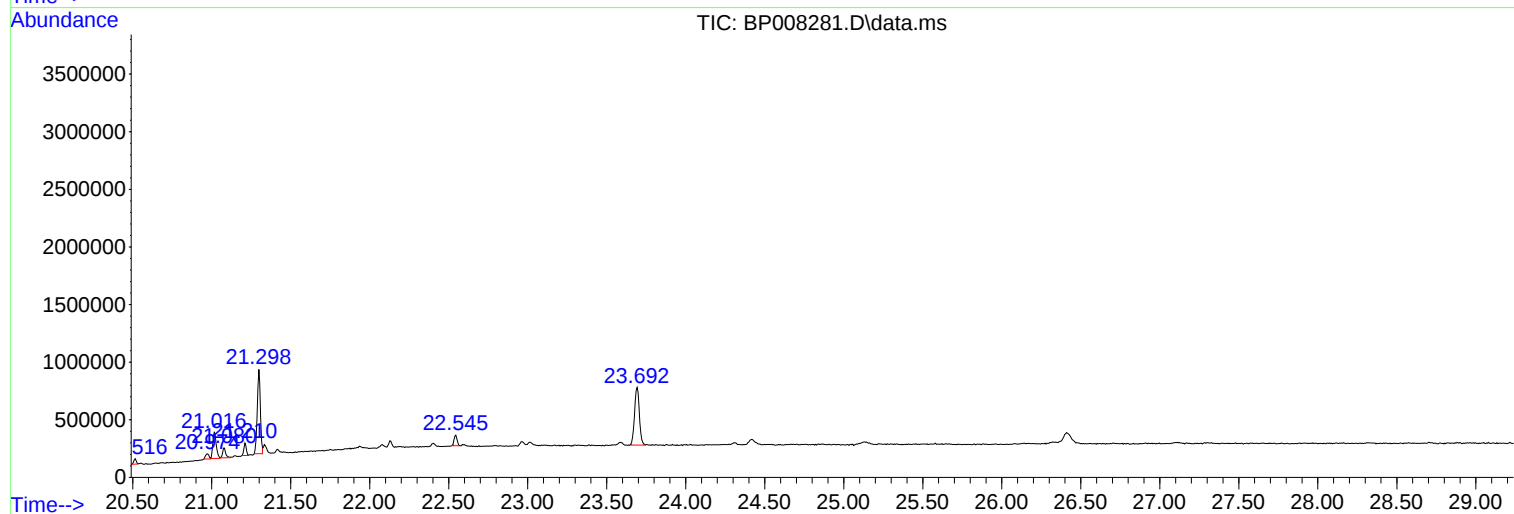
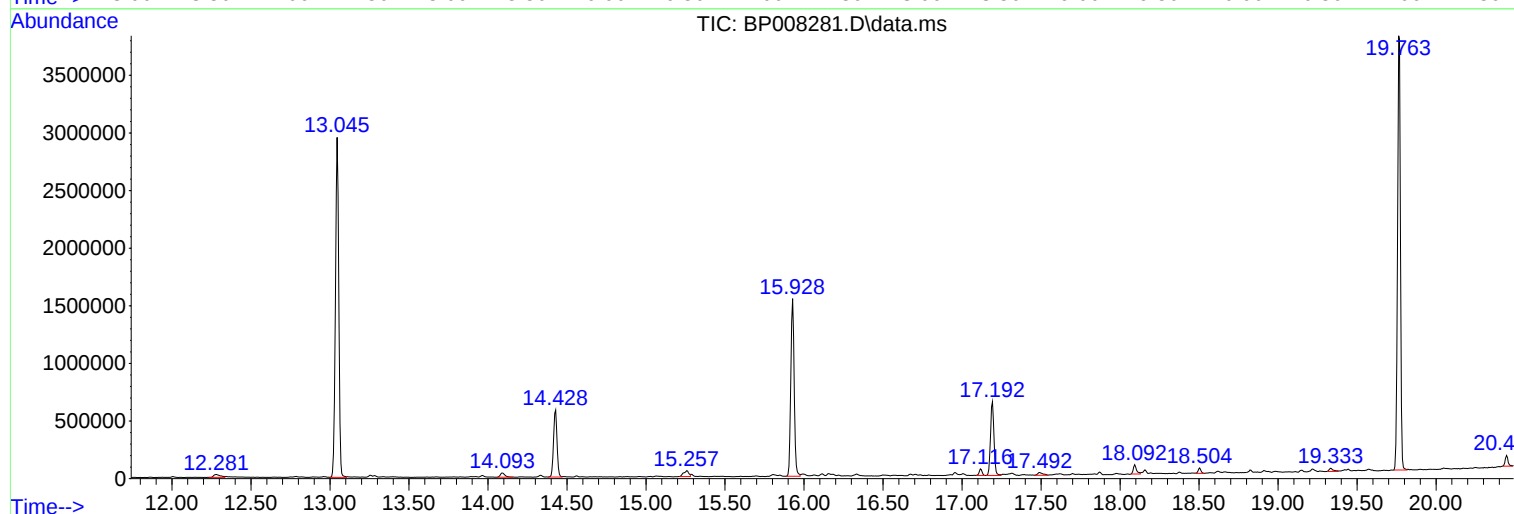
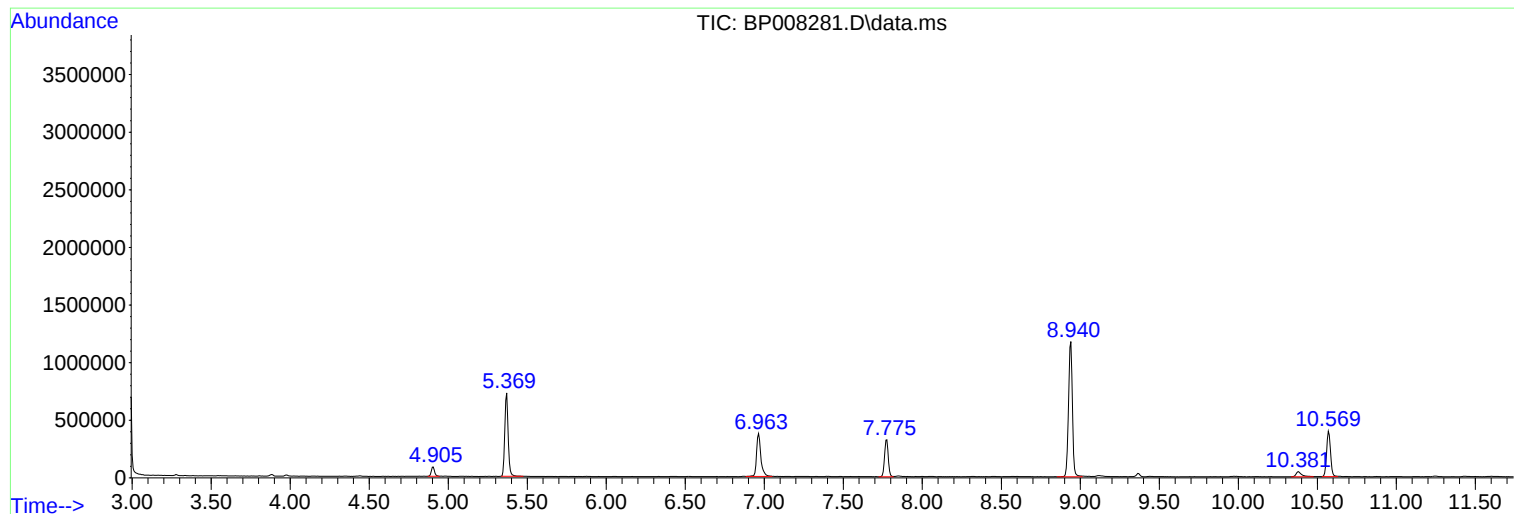
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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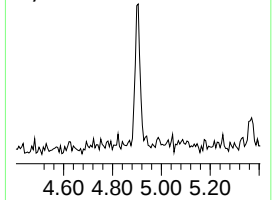
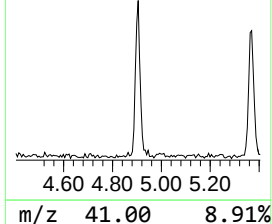
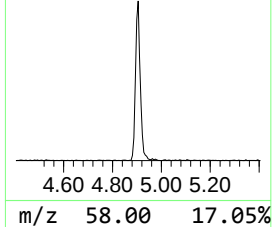
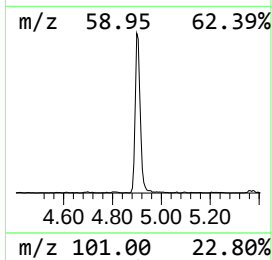
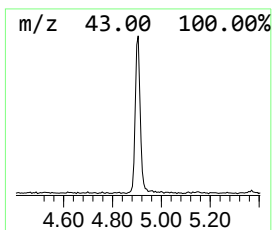
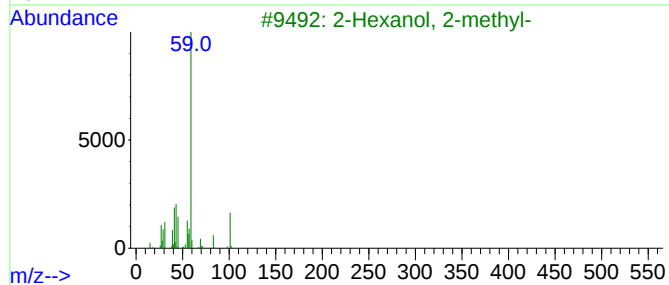
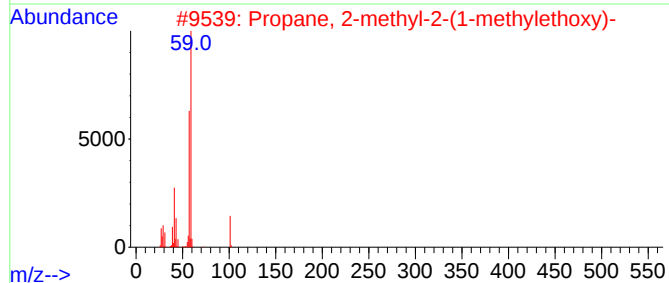
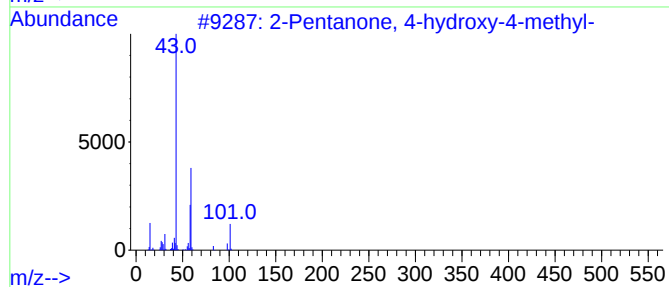
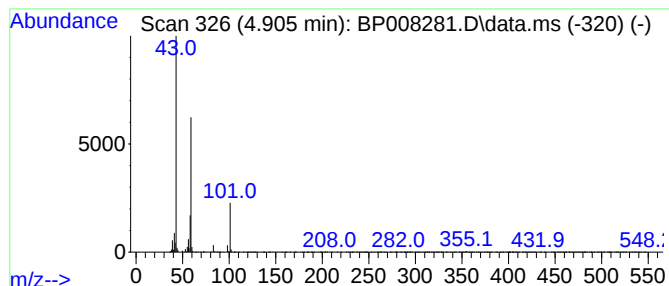
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	4.38 ng	114581	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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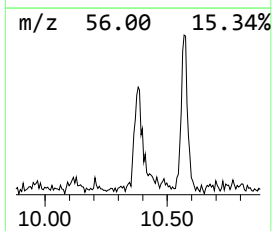
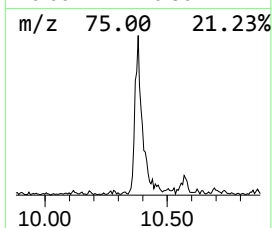
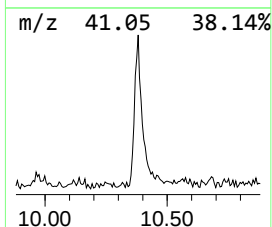
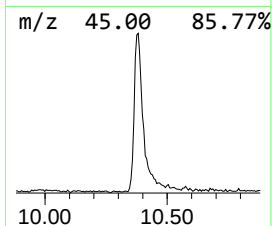
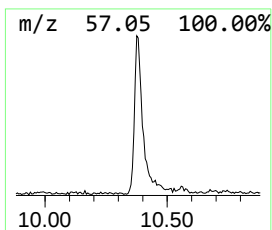
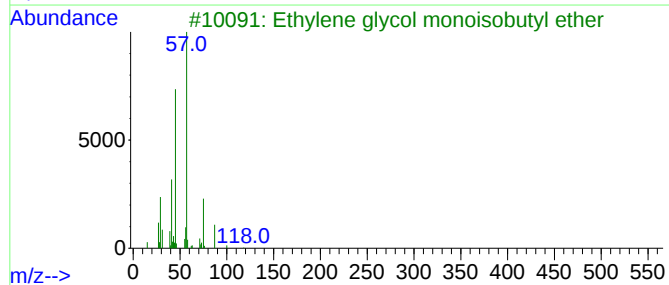
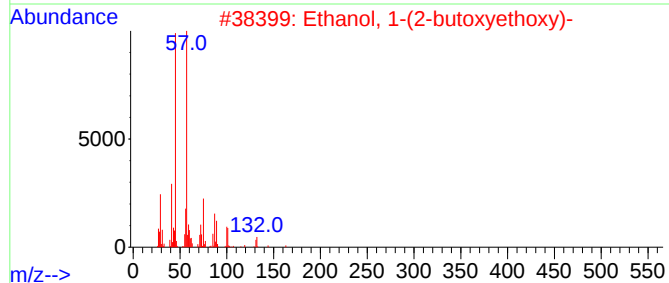
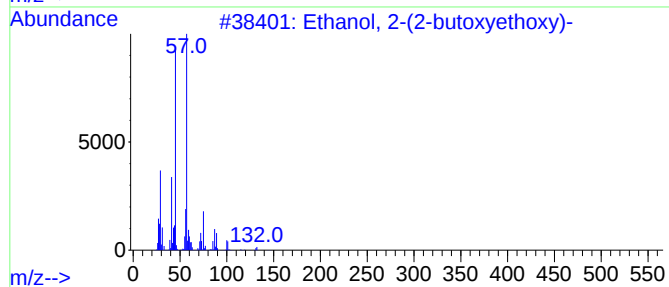
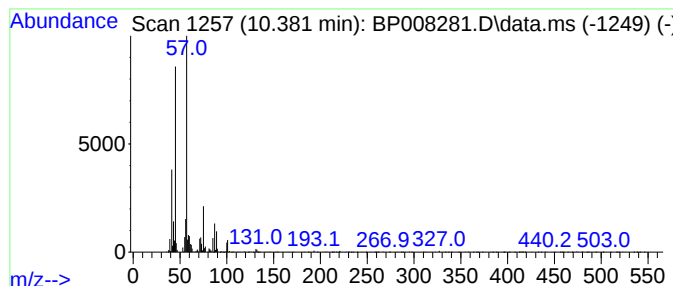
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.381	3.18 ng	107391	Naphthalene-d8	10.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	50
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47



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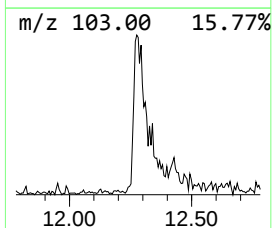
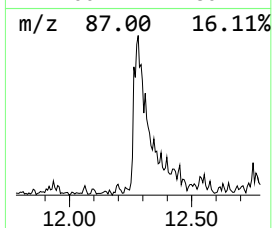
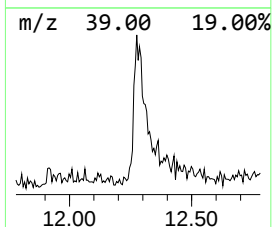
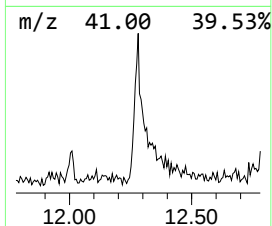
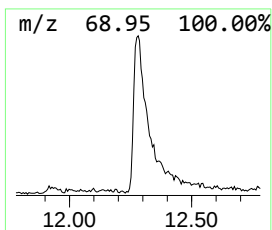
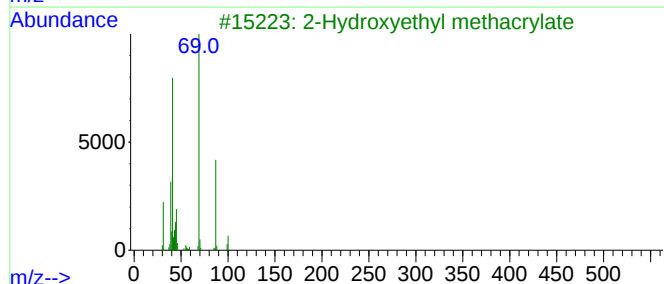
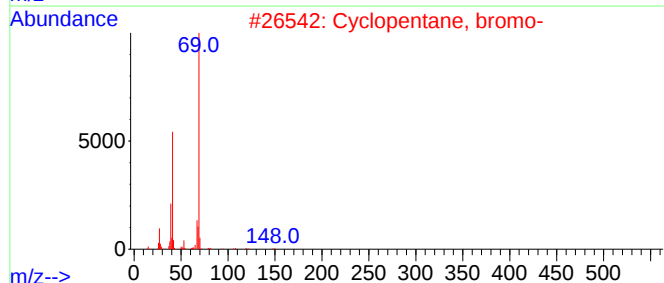
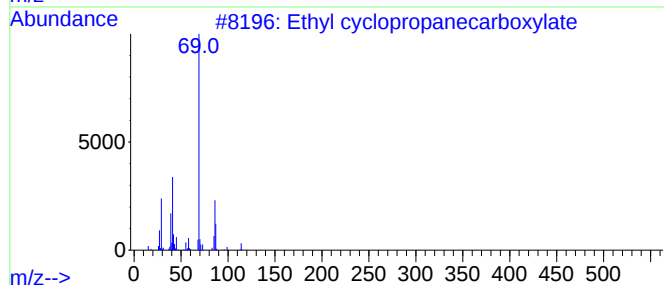
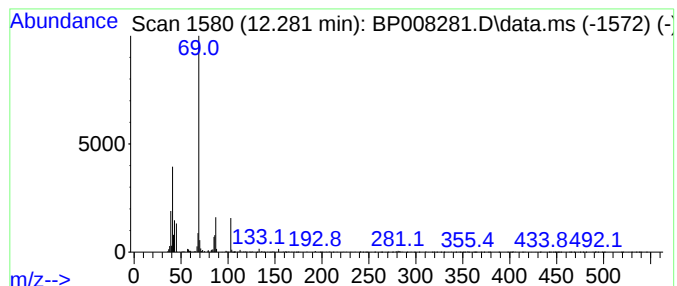
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethyl cyclopropanecarboxylate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.281	2.31 ng	78054	Naphthalene-d8	10.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	50
2			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	49
3			2-Hydroxyethyl methacrylate	130	C6H10O3	000868-77-9	45
4			1-Octyn-4-ol	126	C8H14O	052517-92-7	45
5			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	40



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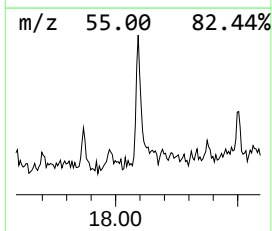
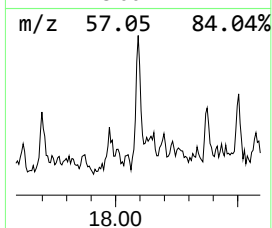
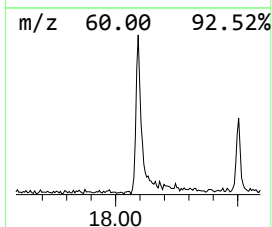
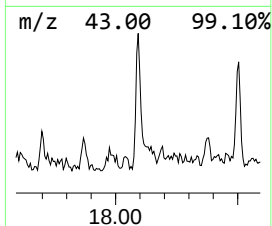
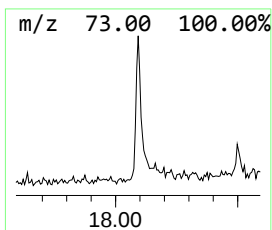
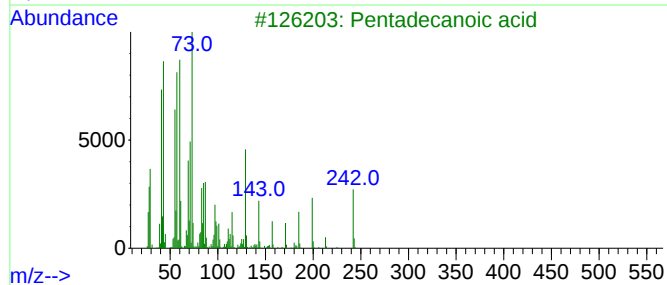
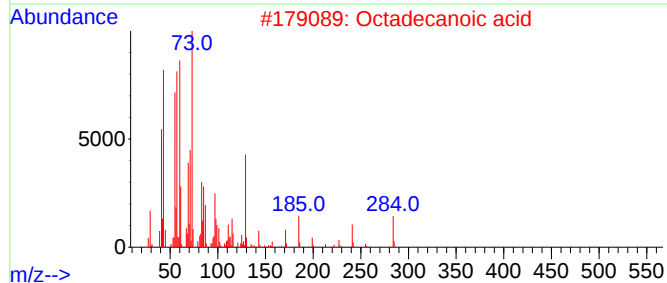
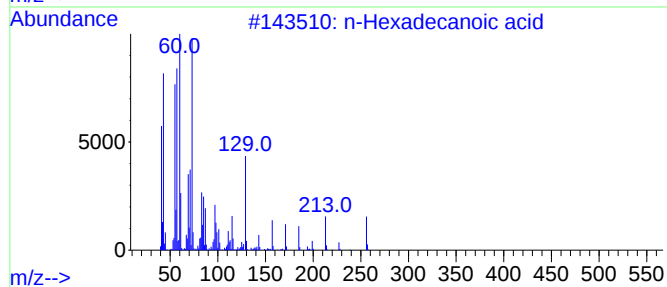
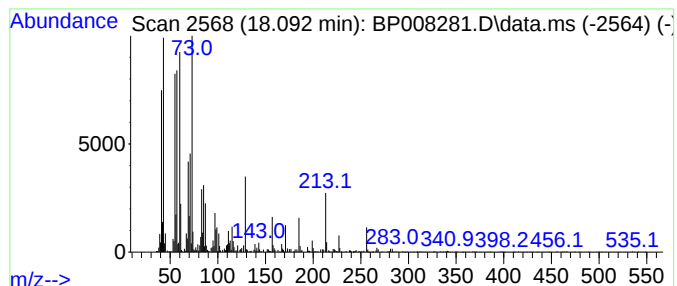
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	2.43 ng	116570	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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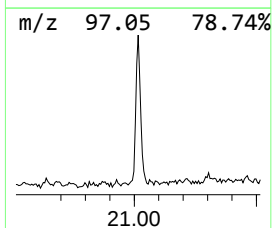
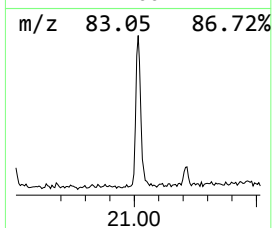
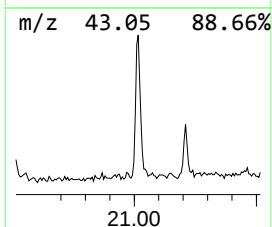
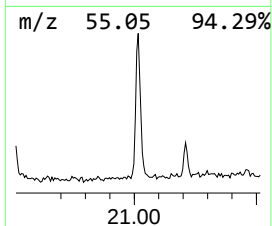
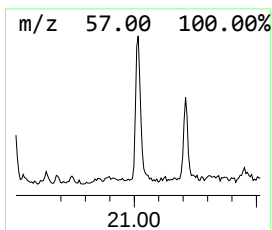
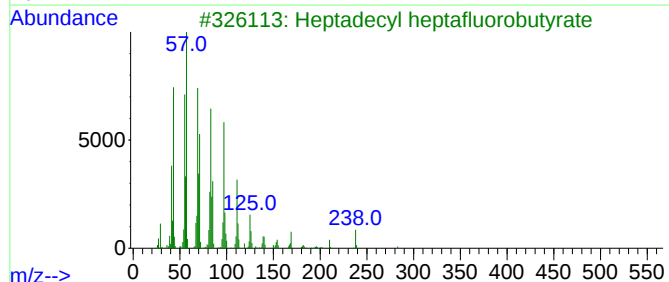
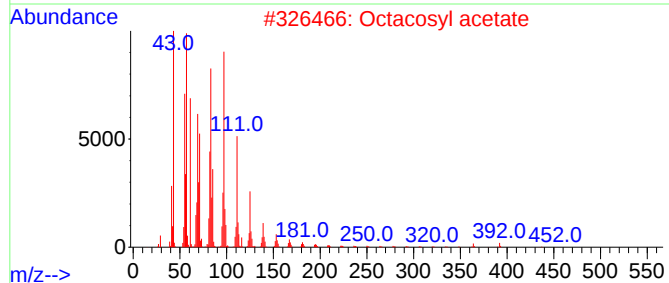
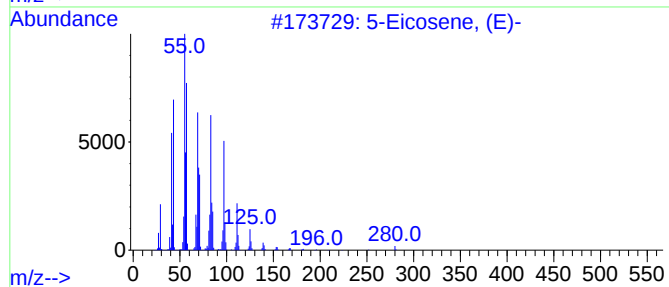
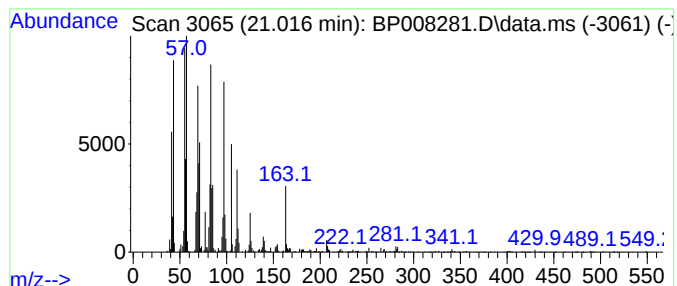
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.016	6.91 ng	346267	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2			Octacosyl acetate	452	C30H60O2	018206-97-8	95
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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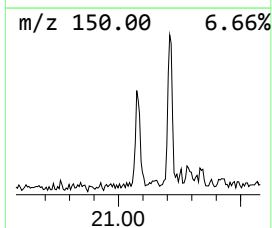
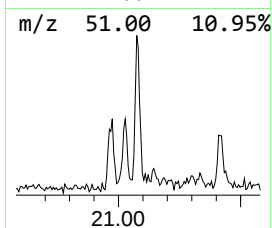
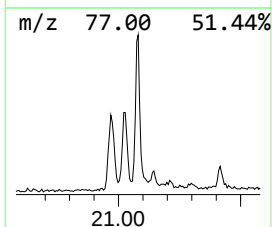
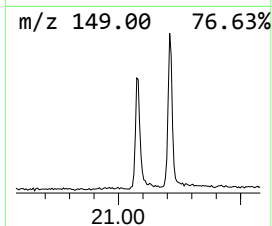
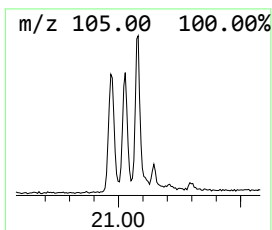
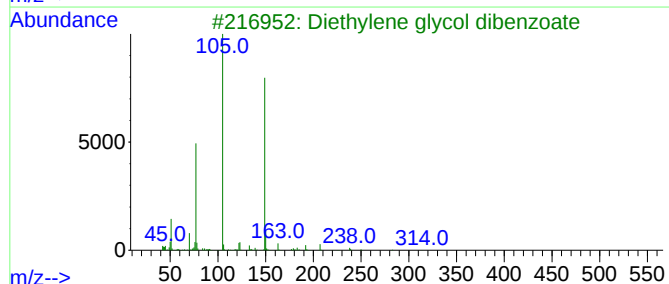
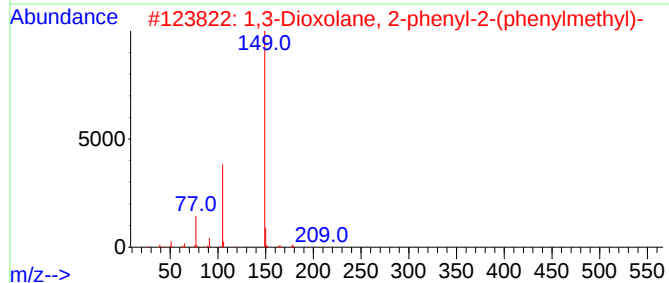
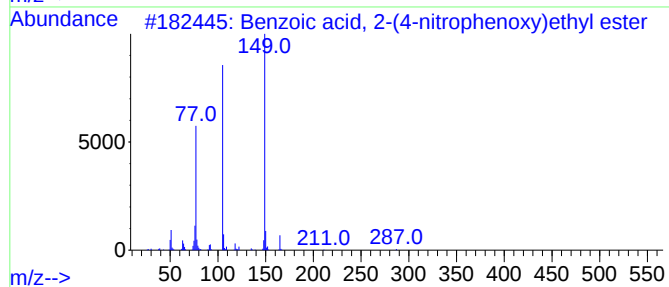
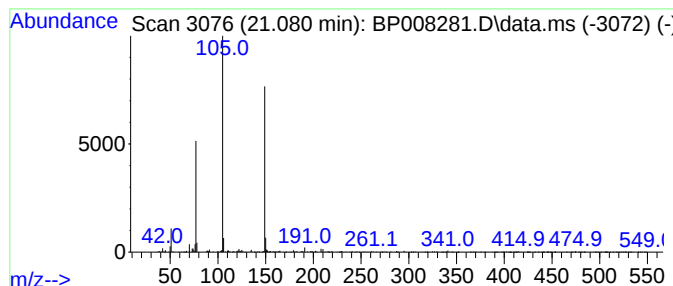
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzoic acid, 2-(4-nitrophe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	2.32 ng	116285	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	80
2			1,3-Dioxolane, 2-phenyl-2-(pheny...	240	C16H16O2	004362-19-0	78
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
4			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
5			N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008281.D
Acq On : 08 Dec 2021 15:34
Operator : CG/JU
Sample : M4953-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A377

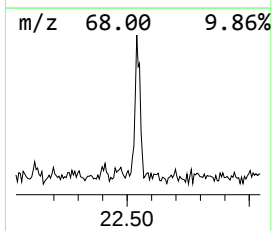
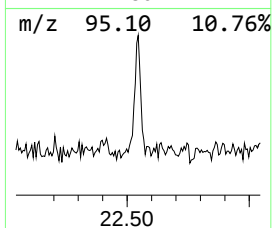
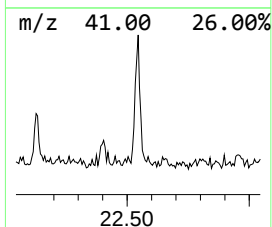
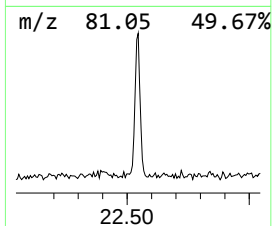
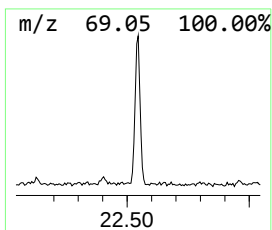
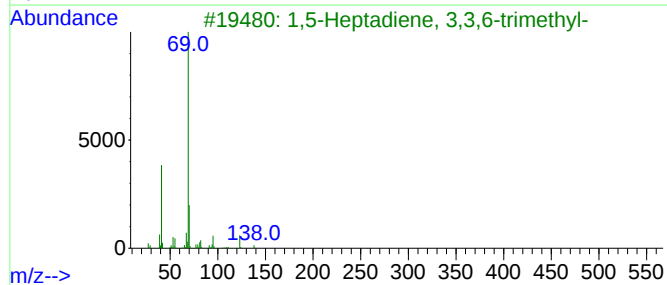
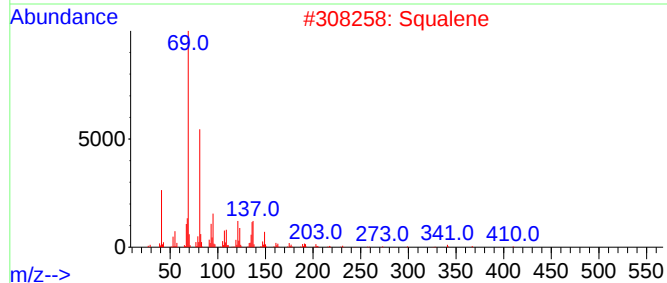
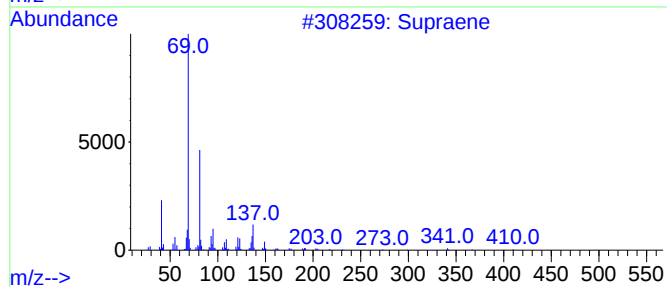
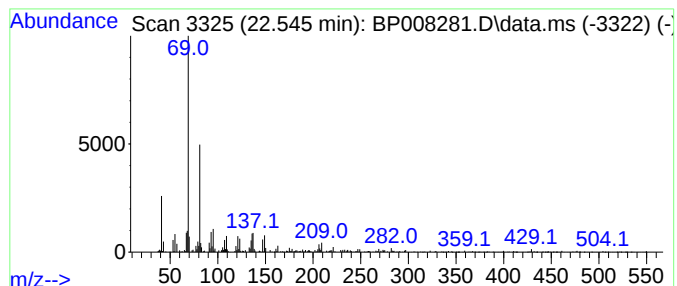
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.545	2.20 ng	115326	Perylene-d12	23.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	98
2			Squalene	410	C30H50	000111-02-4	93
3			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	72
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5			trans-Farnesol	222	C15H26O	000106-28-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008281.D
Acq On : 08 Dec 2021 15:34
Operator : CG/JU
Sample : M4953-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A377

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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-...	4.905	4.4	ng	114581	1	7.775	523411	20.0
Ethanol, 2-(2-b...	10.381	3.2	ng	107391	2	10.569	675285	20.0
Ethyl cycloprop...	12.281	2.3	ng	78054	2	10.569	675285	20.0
n-Hexadecanoic ...	18.092	2.4	ng	116570	4	17.192	958701	20.0
5-Eicosene, (E)-	21.016	6.9	ng	346267	5	21.298	1002820	20.0
Benzoic acid, 2...	21.080	2.3	ng	116285	5	21.298	1002820	20.0
Supraene	22.545	2.2	ng	115326	6	23.692	1046970	20.0