

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
 Data File : BF131020.D
 Acq On : 05 Nov 2022 15:24
 Operator : CG\JU
 Sample : N5335-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2

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_F\Methods\8270-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131020.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	12	19	25	rVB	458264	600991	29.56%	4.305%
2	5.128	512	517	527	rVB	233539	292128	14.37%	2.093%
3	5.522	579	584	587	rBV	1776488	1688652	83.06%	12.096%
4	6.528	750	755	758	rBV	1791357	1716405	84.42%	12.295%
5	6.904	815	819	822	rBV	521067	435739	21.43%	3.121%
6	7.469	909	915	917	rBV	1095108	1114064	54.80%	7.980%
7	8.087	1017	1020	1033	rBV	37291	68144	3.35%	0.488%
8	8.187	1033	1037	1040	rVV	633881	518930	25.52%	3.717%
9	9.263	1215	1220	1223	rBV	2259017	2033134	100.00%	14.564%
10	9.945	1332	1336	1340	rBV	797439	621618	30.57%	4.453%
11	10.739	1466	1471	1474	rBV	1469659	1292197	63.56%	9.256%
12	11.439	1586	1590	1593	rBV	753413	599226	29.47%	4.292%
13	11.504	1598	1601	1605	rVB	33874	24841	1.22%	0.178%
14	13.027	1856	1860	1864	rBV	1998018	1784929	87.79%	12.786%
15	13.969	2015	2020	2032	rBV6	33907	98776	4.86%	0.708%
16	14.063	2032	2036	2037	rBV	20597	21487	1.06%	0.154%
17	14.086	2037	2040	2043	rVB	468484	404387	19.89%	2.897%
18	14.180	2051	2056	2061	rBV	67754	74161	3.65%	0.531%
19	15.216	2229	2232	2238	rVB3	22235	28113	1.38%	0.201%
20	15.586	2290	2295	2303	rVB2	300794	394305	19.39%	2.825%
21	16.057	2371	2375	2380	rBV2	23696	33480	1.65%	0.240%
22	16.598	2459	2467	2470	rBV3	21571	41965	2.06%	0.301%
23	17.204	2565	2570	2578	rBV5	17156	39820	1.96%	0.285%
24	17.951	2690	2697	2704	rVB5	13975	32421	1.59%	0.232%

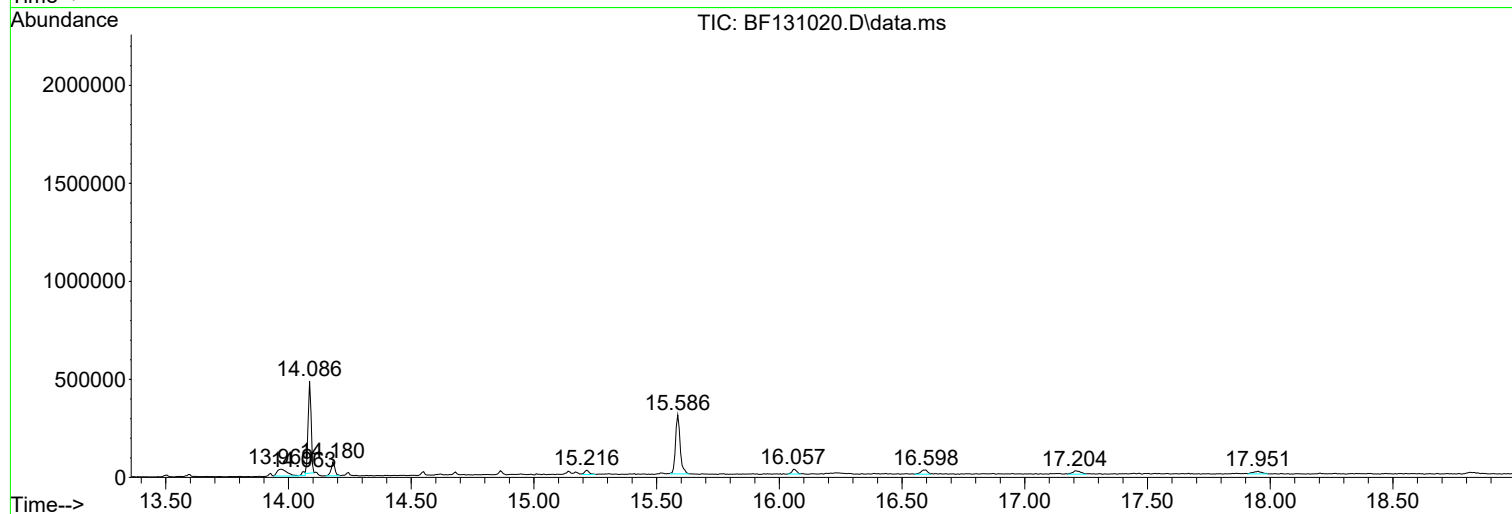
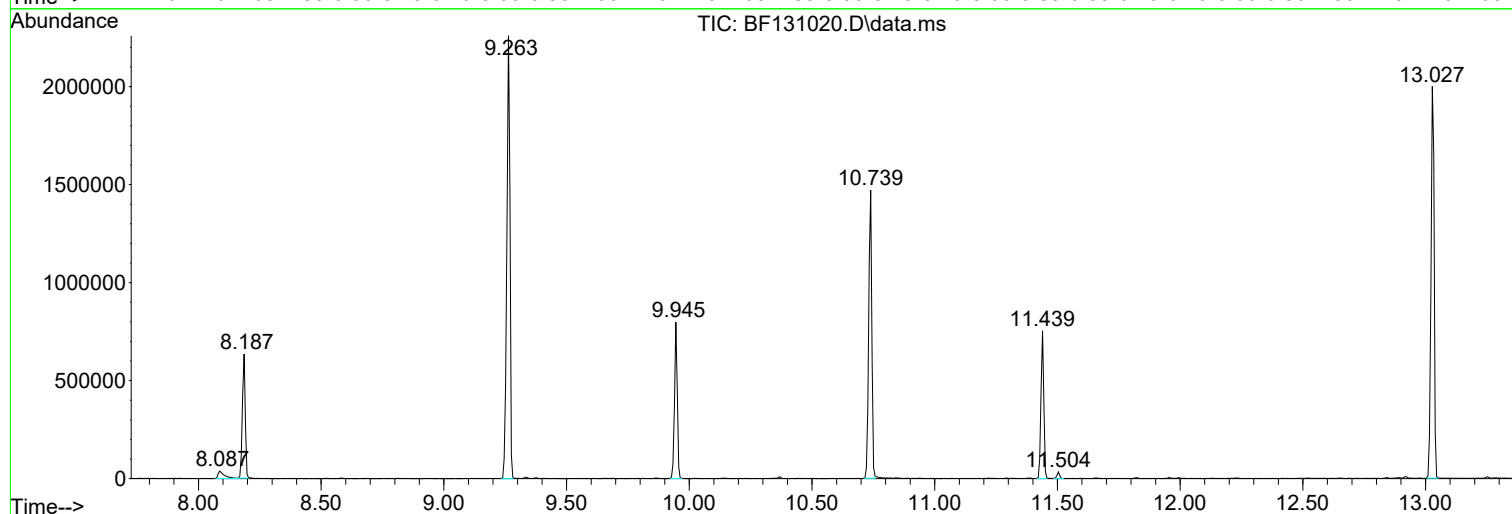
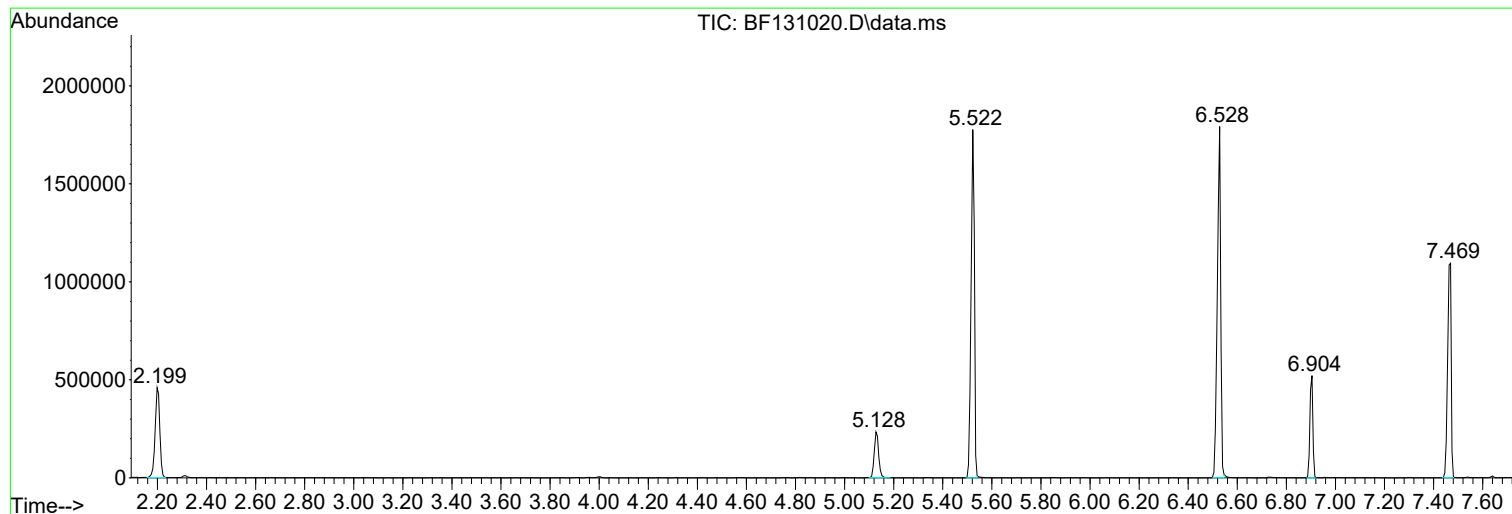
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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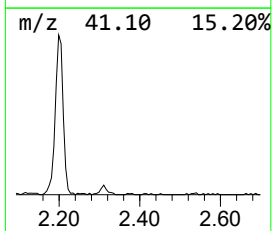
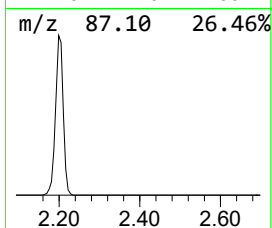
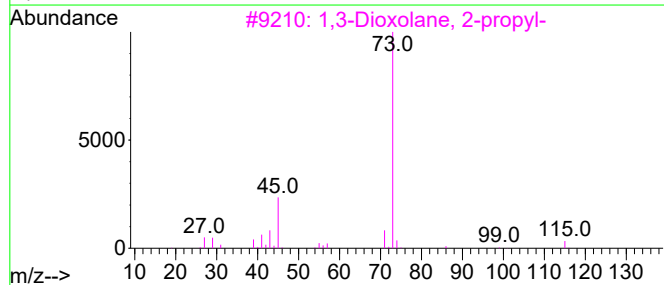
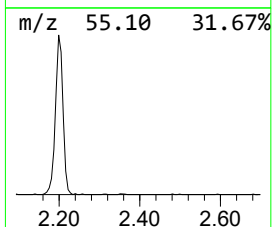
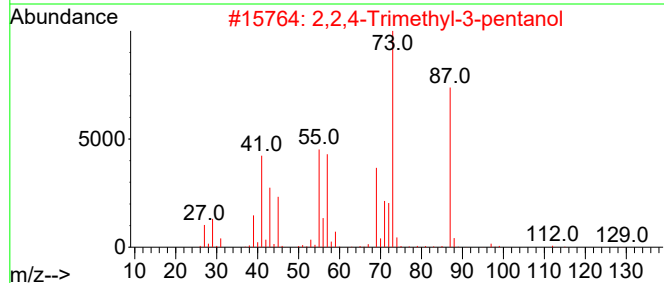
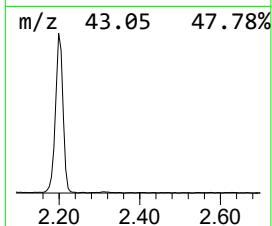
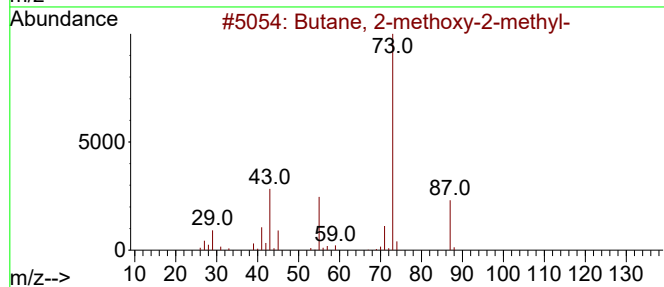
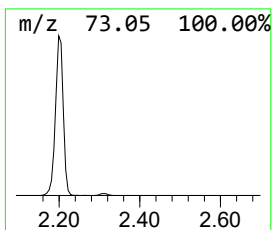
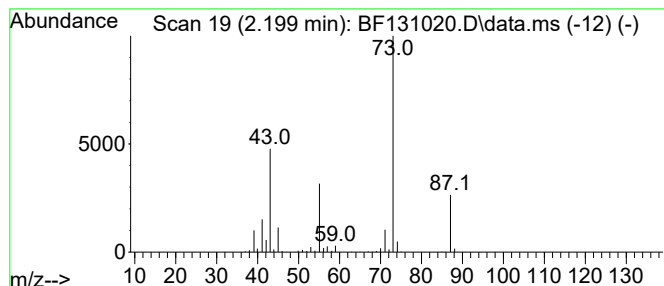
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	27.58 ng	600991	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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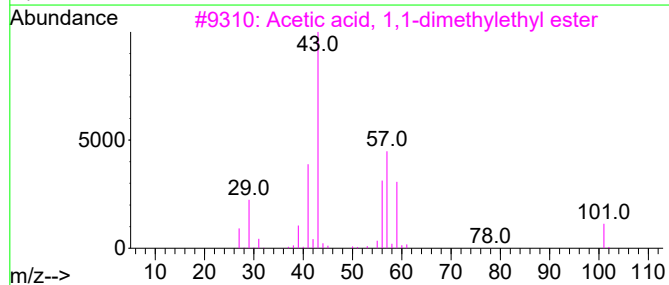
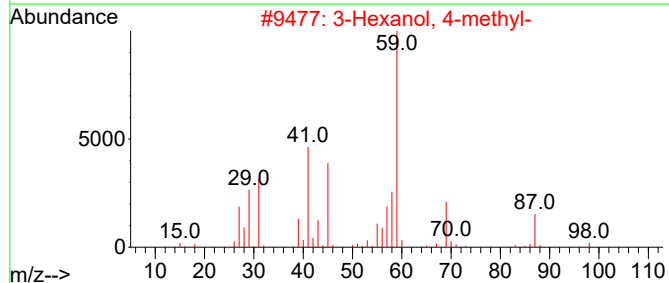
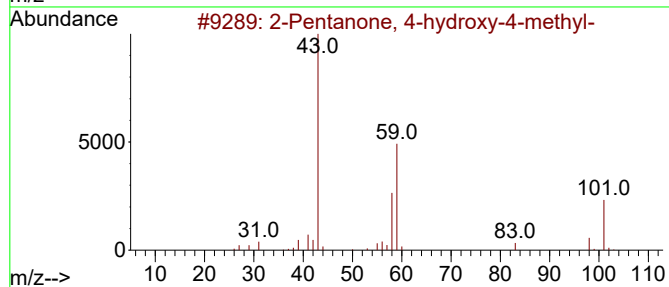
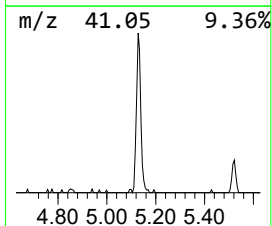
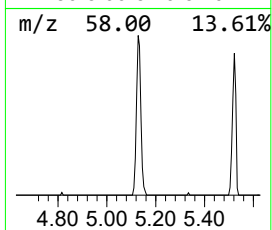
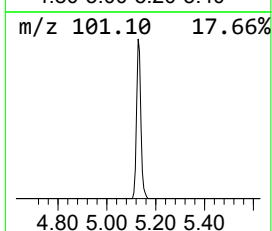
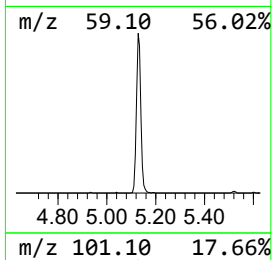
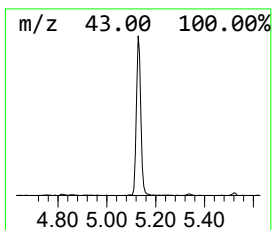
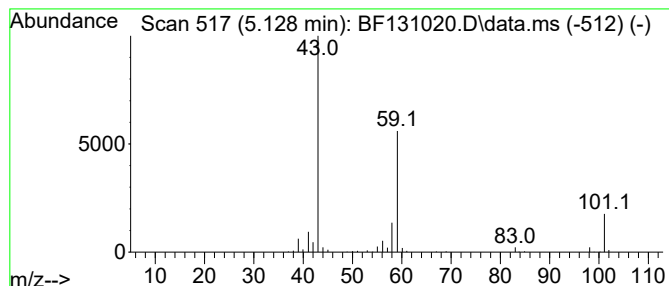
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	13.41 ng	292128	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
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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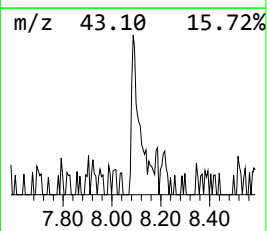
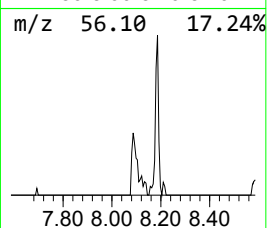
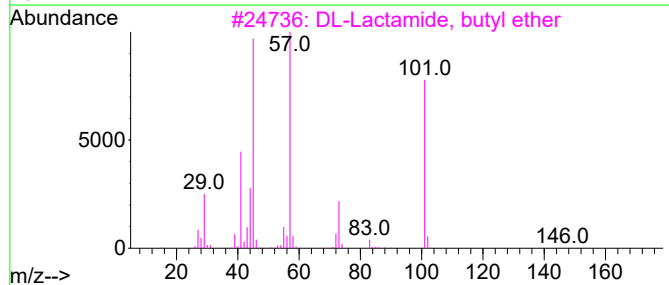
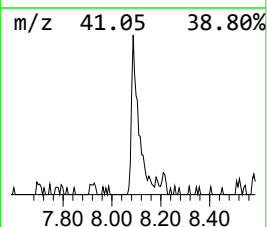
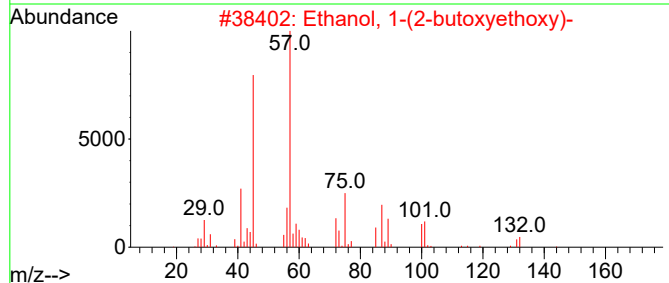
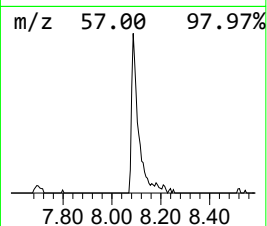
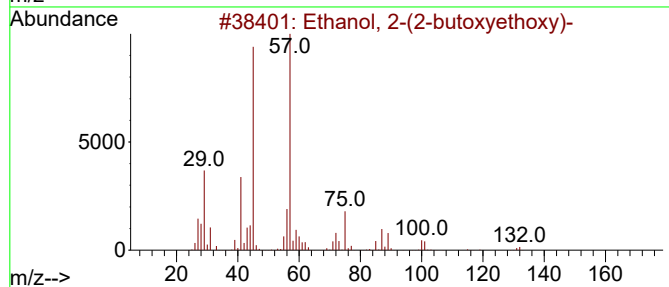
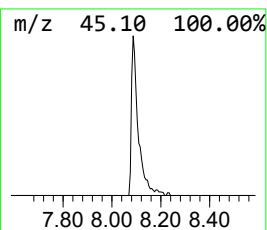
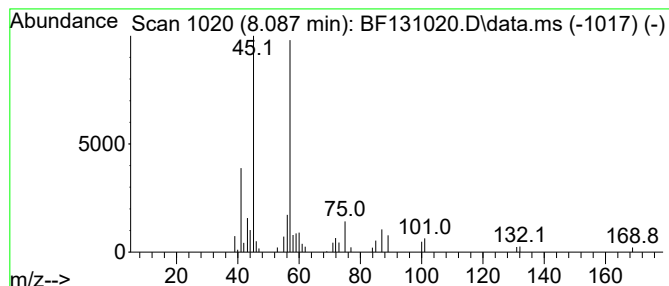
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.087	2.63 ng	68144	Naphthalene-d8	8.187

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			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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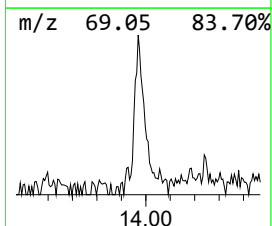
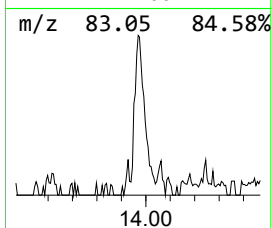
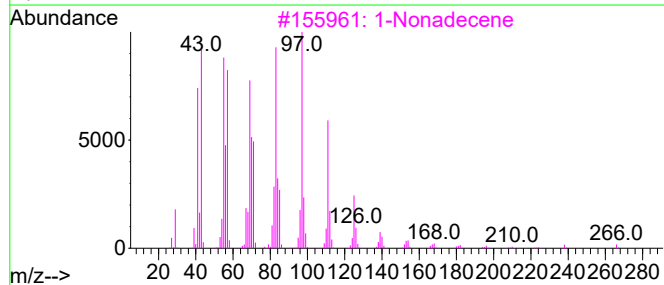
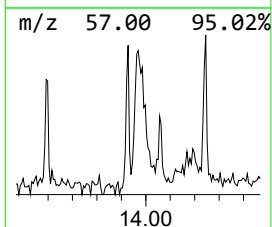
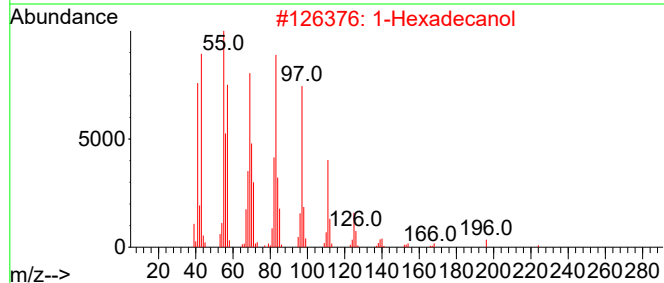
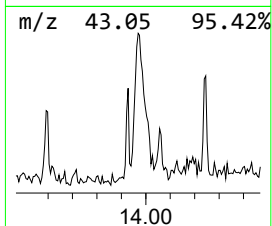
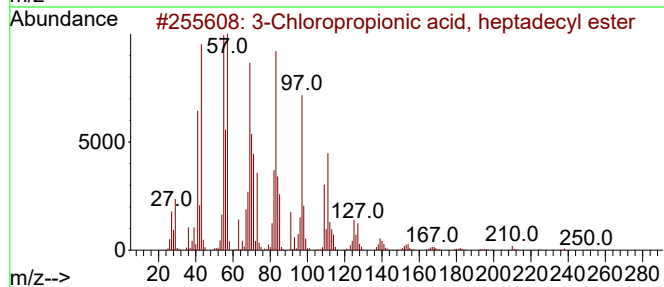
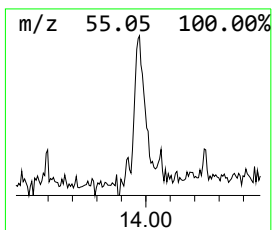
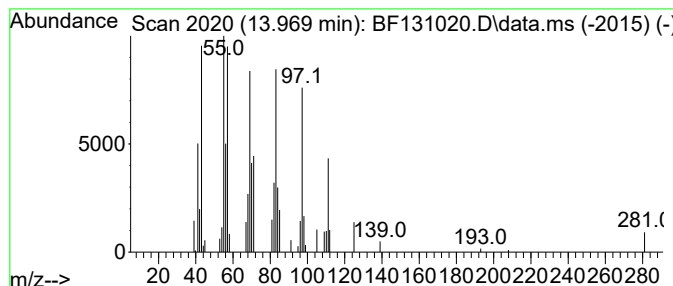
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Peak Number 4 3-Chloropropionic acid, hep... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	4.89 ng	98776	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
2			1-Hexadecanol	242	C16H34O	036653-82-4	93
3			1-Nonadecene	266	C19H38	018435-45-5	91
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5			1-Heneicosanol	312	C21H44O	015594-90-8	90



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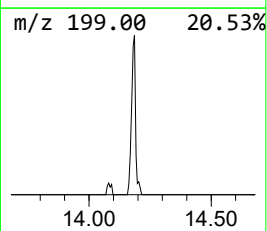
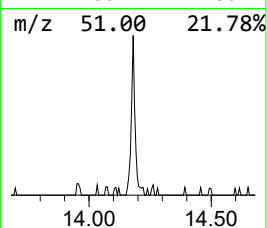
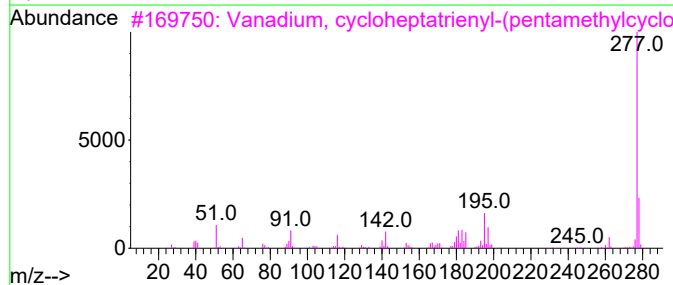
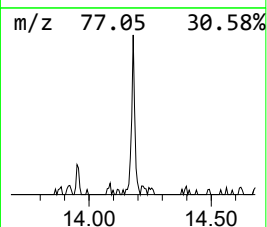
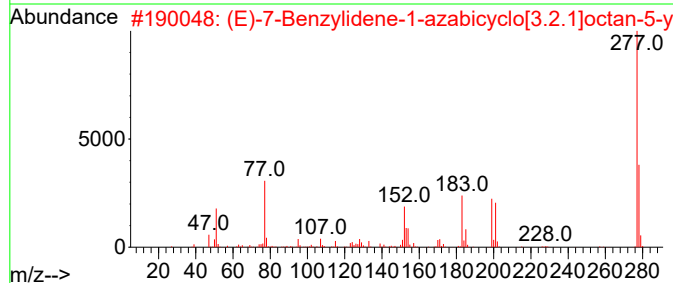
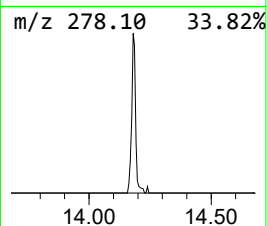
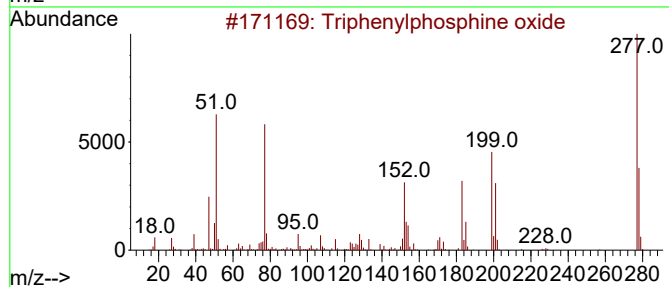
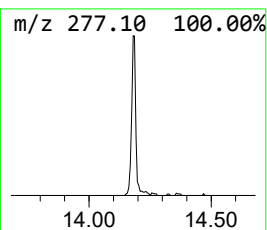
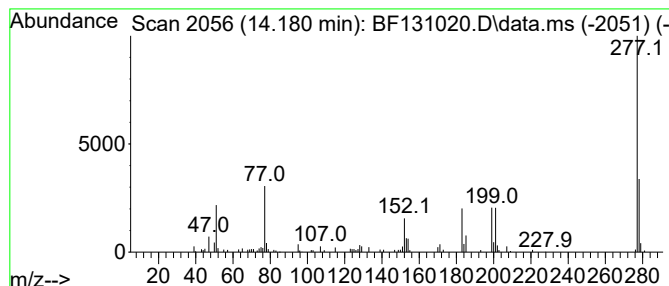
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.180	3.67 ng	74161	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3.1.0]octan-5-yl	293	C15H19NO3S	1000483-83-4	90
3			Vanadium, cycloheptatrienyl-(pentamethylcyclopentadienyl)-	277	C17H22V	1000155-20-5	32
4			3-(3,4-Dichlorophenyl)-2-thioxo-1,2,3,4-tetrahydronaphthalene	277	C9H5Cl2NOS2	017046-34-3	25
5			Carbazol-1-one, 1,2,3,4-tetrahydronaphthalen-1-yl	277	C18H15NO2	299962-12-2	25



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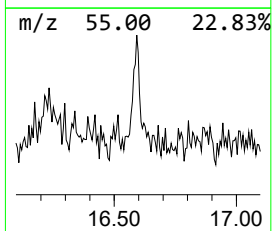
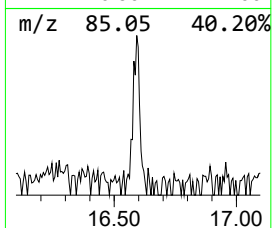
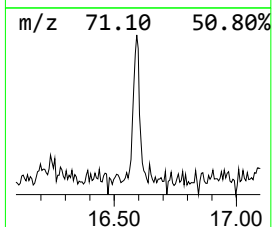
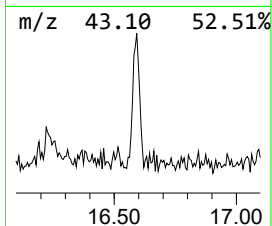
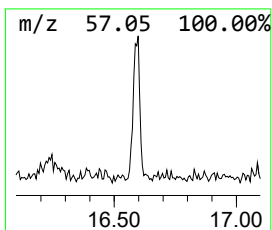
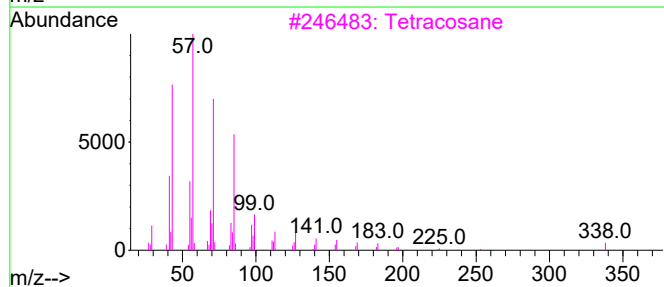
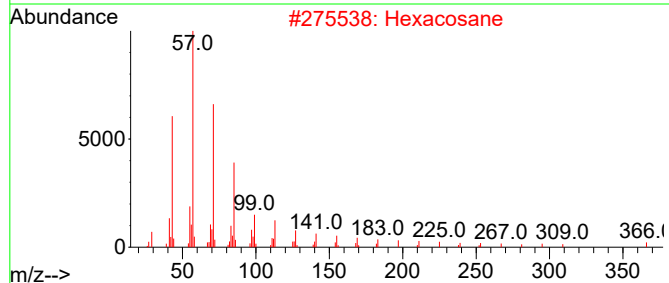
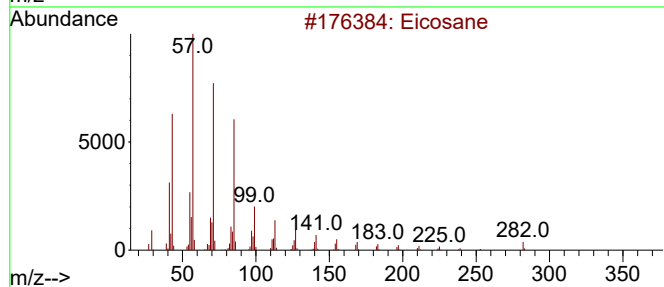
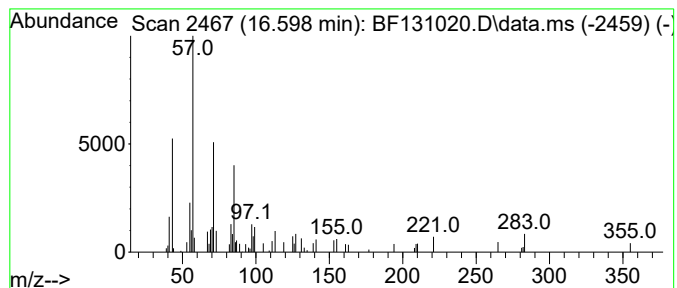
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.598	2.13 ng	41965	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	95
2	Hexacosane			366	C26H54	000630-01-3	68
3	Tetracosane			338	C24H50	000646-31-1	68
4	Hentriacontane			437	C31H64	000630-04-6	68
5	Pentacosane			352	C25H52	000629-99-2	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131020.D
Acq On : 05 Nov 2022 15:24
Operator : CG\JU
Sample : N5335-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2

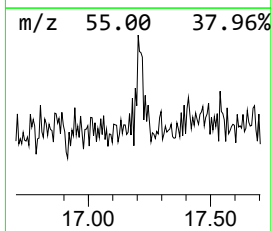
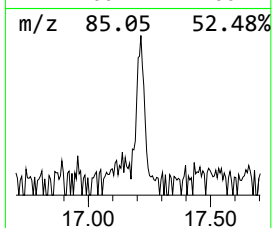
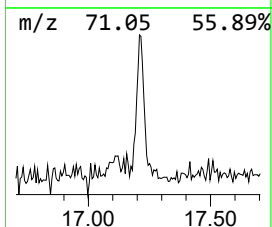
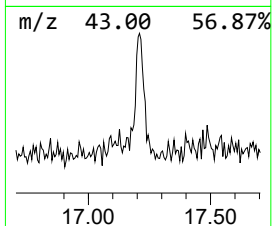
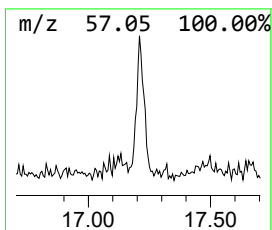
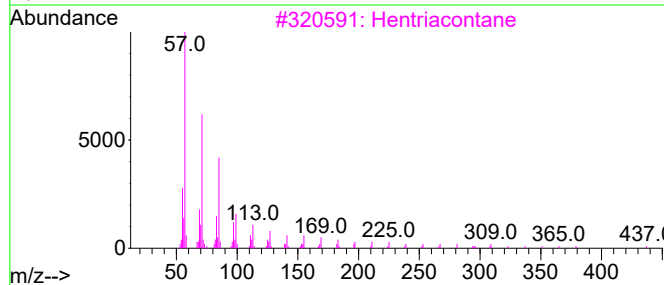
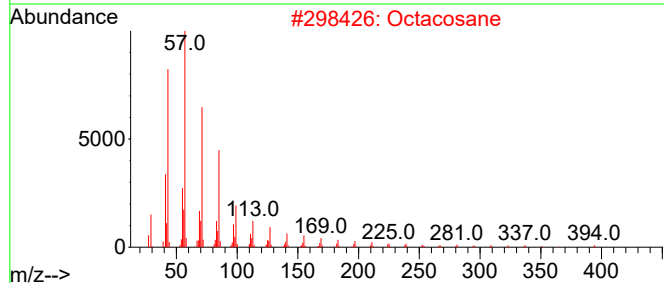
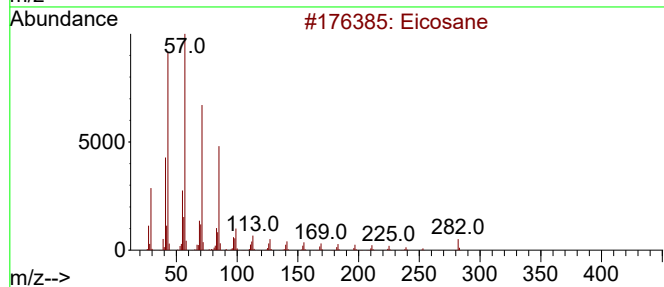
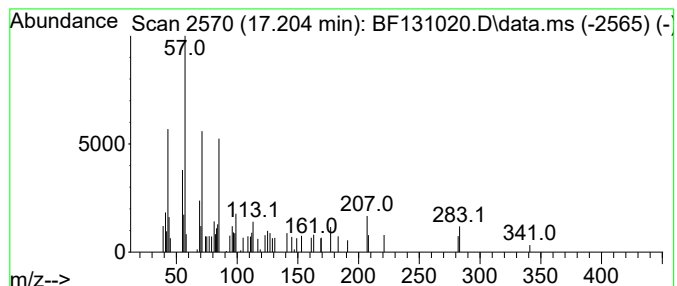
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.204	2.02 ng	39820	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	92
2	Octacosane			394	C28H58	000630-02-4	53
3	Hentriacontane			437	C31H64	000630-04-6	52
4	Pentacosane			352	C25H52	000629-99-2	49
5	Tetracosane			338	C24H50	000646-31-1	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131020.D
Acq On : 05 Nov 2022 15:24
Operator : CG\JU
Sample : N5335-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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
Butane, 2-metho...	2.199	27.6	ng	600991	1	6.904	435739	20.0
2-Pentanone, 4-...	5.128	13.4	ng	292128	1	6.904	435739	20.0
Ethanol, 2-(2-b...	8.087	2.6	ng	68144	2	8.187	518930	20.0
3-Chloropropion...	13.969	4.9	ng	98776	5	14.086	404387	20.0
Triphenylphosph...	14.180	3.7	ng	74161	5	14.086	404387	20.0
Eicosane	16.598	2.1	ng	41965	6	15.586	394305	20.0
Octacosane	17.204	2.0	ng	39820	6	15.586	394305	20.0