

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
 Data File : BF130989.D
 Acq On : 04 Nov 2022 13:25
 Operator : CG\JU
 Sample : N5272-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20221104-COMP-03

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: BF130989.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.281	25	33	39	rVB	1234203	1606691	60.02%	7.469%
2	2.387	47	51	56	rVB	48238	57483	2.15%	0.267%
3	5.151	517	521	532	rVB	296315	371687	13.89%	1.728%
4	5.540	582	587	590	rBV	2655712	2574212	96.17%	11.966%
5	6.534	751	756	769	rVB	1957569	2390355	89.30%	11.112%
6	6.910	816	820	824	rBV	860382	712514	26.62%	3.312%
7	7.475	910	916	919	rBV	1426953	1595729	59.61%	7.418%
8	8.110	1017	1024	1034	rBV2	45992	121752	4.55%	0.566%
9	8.198	1034	1039	1042	rVB	792823	794303	29.67%	3.692%
10	9.275	1216	1222	1225	rBV	2612290	2676836	100.00%	12.443%
11	9.957	1333	1338	1342	rVB	991472	977780	36.53%	4.545%
12	10.751	1466	1473	1477	rBV	2118240	2025710	75.68%	9.417%
13	11.327	1566	1571	1576	rVB2	32360	35548	1.33%	0.165%
14	11.451	1587	1592	1596	rBV	1051319	940738	35.14%	4.373%
15	11.516	1600	1603	1606	rVB	67269	54042	2.02%	0.251%
16	12.239	1718	1726	1732	rBV3	28680	49346	1.84%	0.229%
17	13.045	1858	1863	1866	rBV	2793820	2460834	91.93%	11.439%
18	13.610	1954	1959	1961	rBV2	32523	32272	1.21%	0.150%
19	13.939	2011	2015	2018	rBV	42540	36818	1.38%	0.171%
20	14.016	2021	2028	2036	rBV3	62082	194822	7.28%	0.906%
21	14.104	2039	2043	2046	rVB	989755	807217	30.16%	3.752%
22	14.198	2053	2059	2063	rBV	89660	117456	4.39%	0.546%
23	14.257	2065	2069	2072	rBV	40905	45146	1.69%	0.210%
24	14.563	2118	2121	2124	rBV	43526	36522	1.36%	0.170%
25	14.880	2171	2175	2181	rBV	42604	41097	1.54%	0.191%
26	14.957	2182	2188	2194	rVV	76890	102558	3.83%	0.477%
27	15.233	2231	2235	2240	rBV	33557	43501	1.63%	0.202%
28	15.610	2294	2299	2306	rVB	442557	578139	21.60%	2.687%
29	16.086	2377	2380	2385	rVB2	20905	31203	1.17%	0.145%

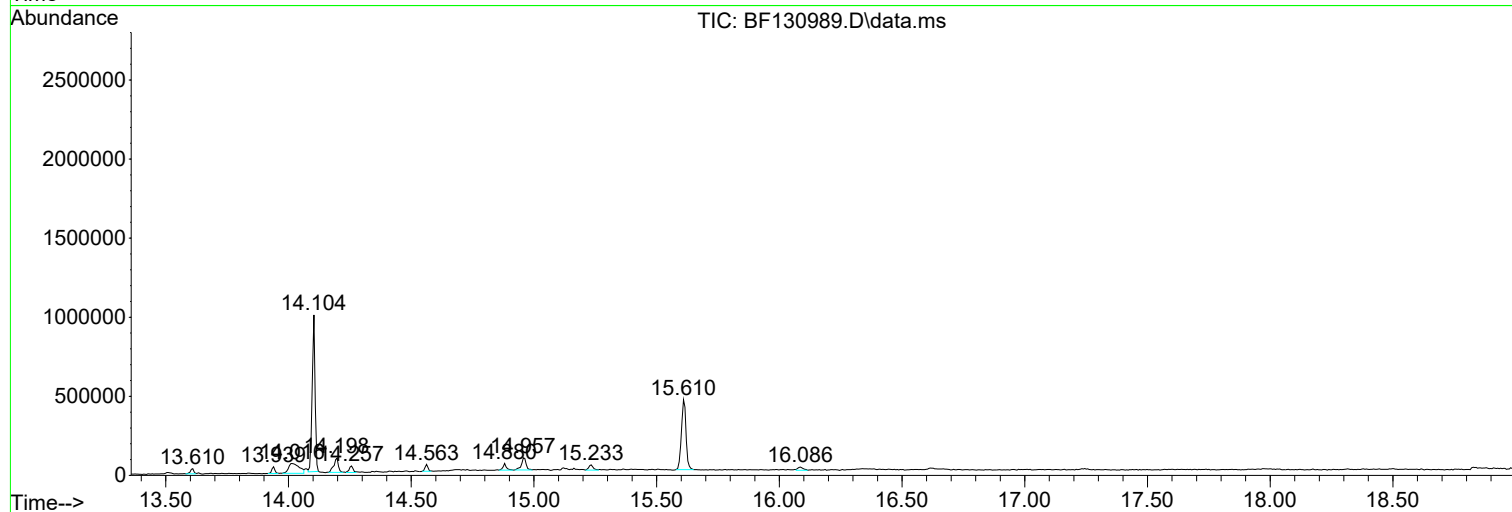
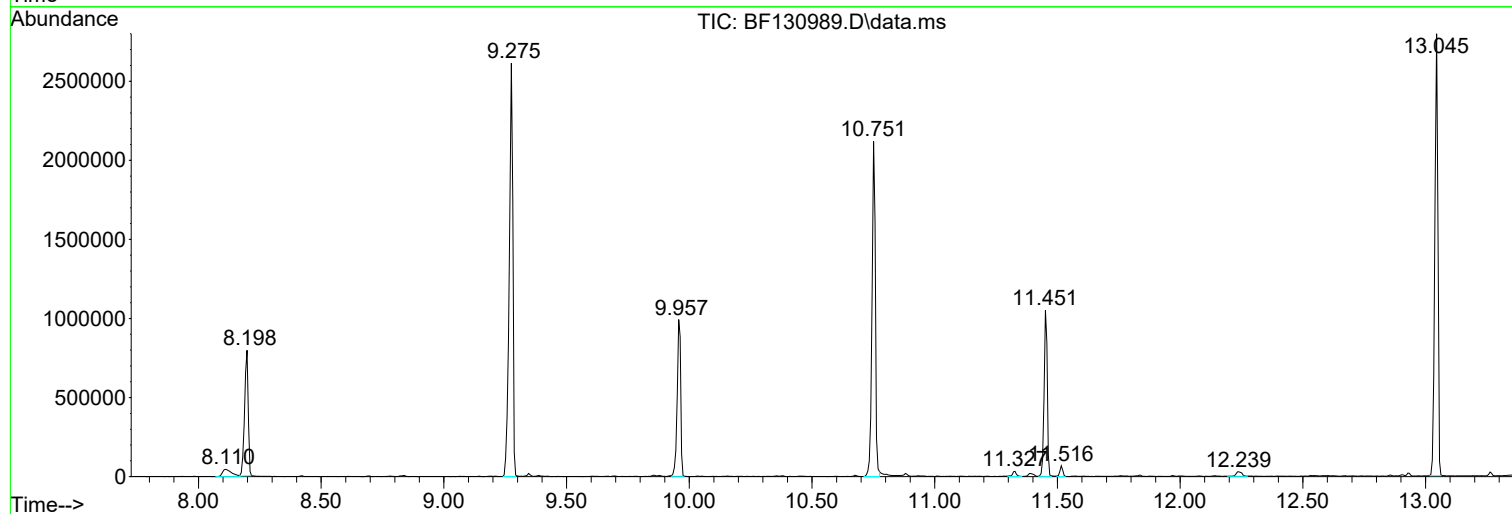
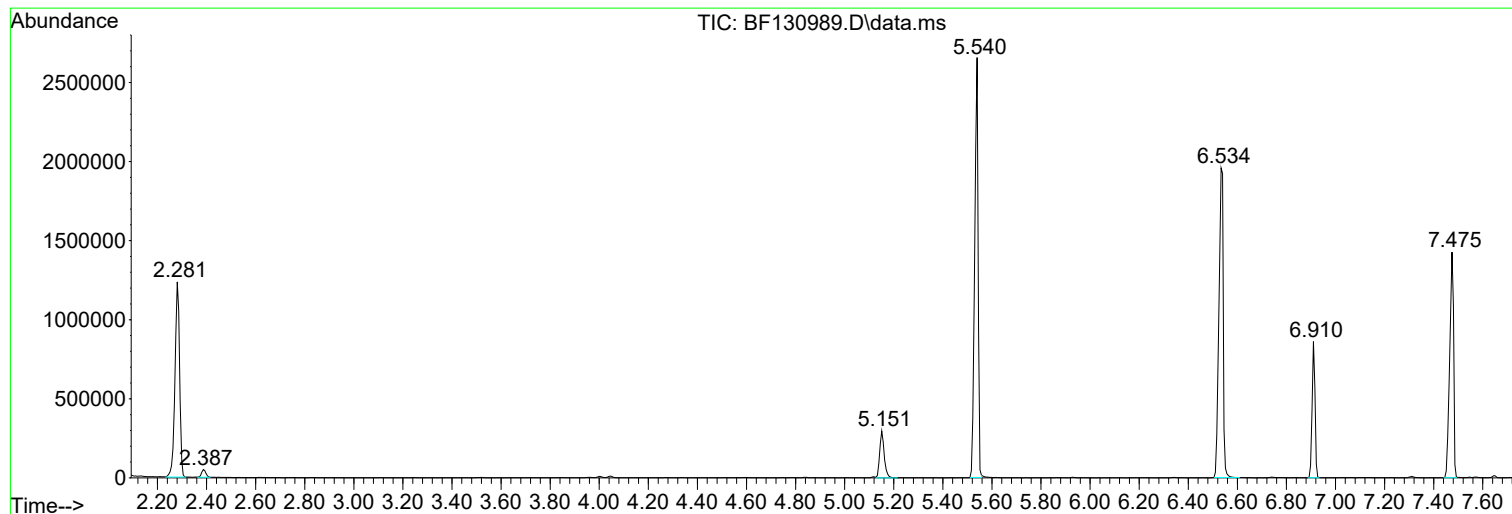
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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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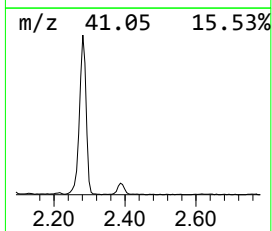
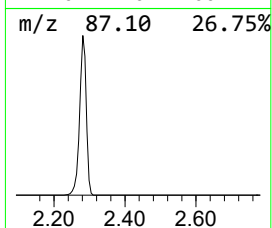
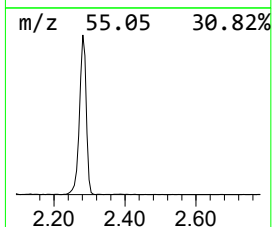
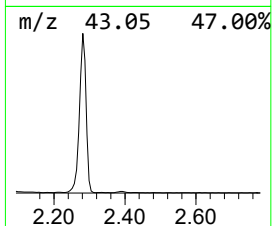
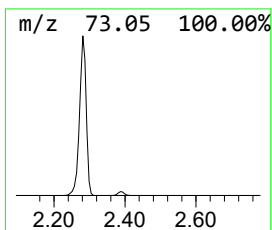
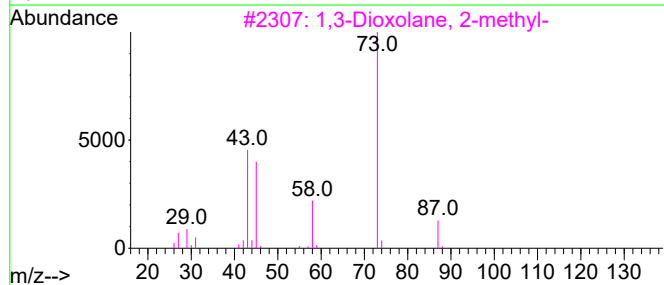
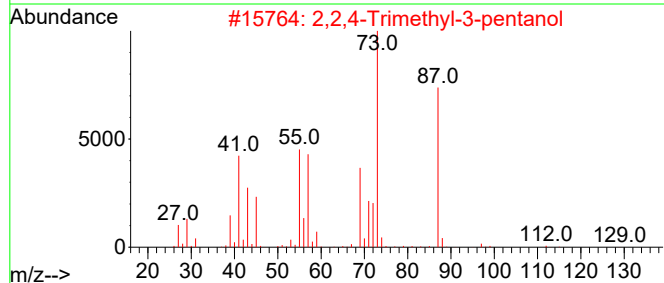
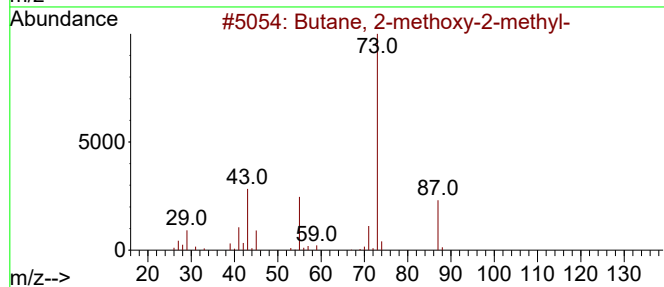
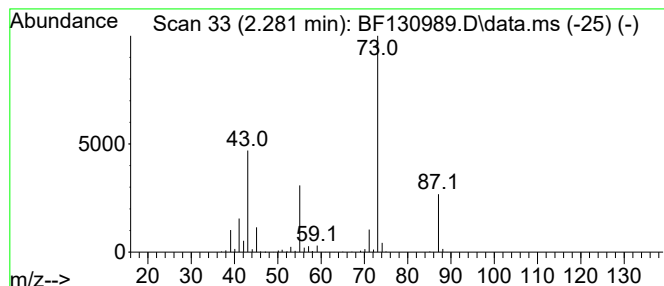
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	45.10 ng	1606690	1,4-Dichlorobenzene-d4	6.910

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-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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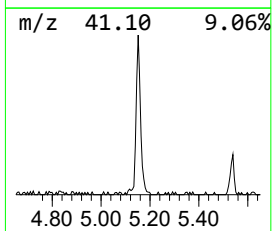
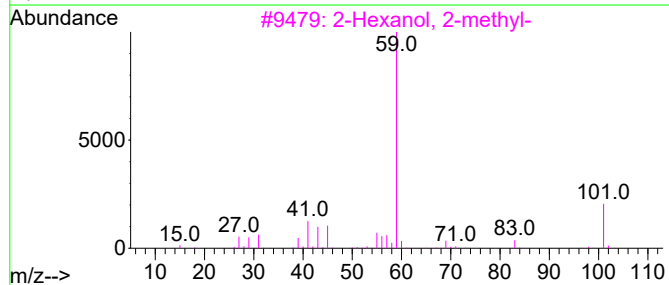
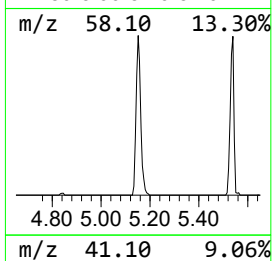
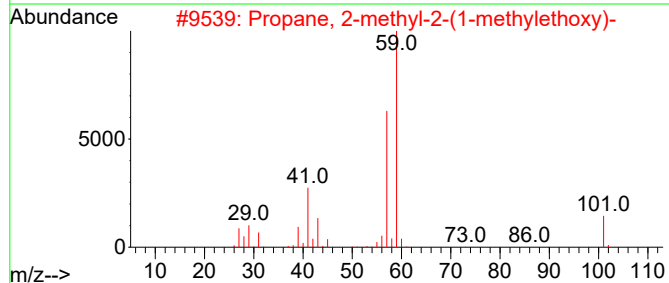
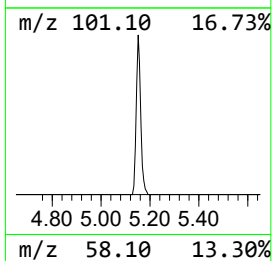
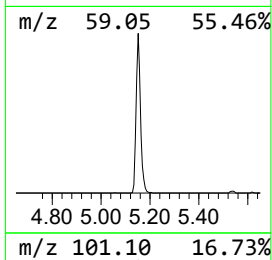
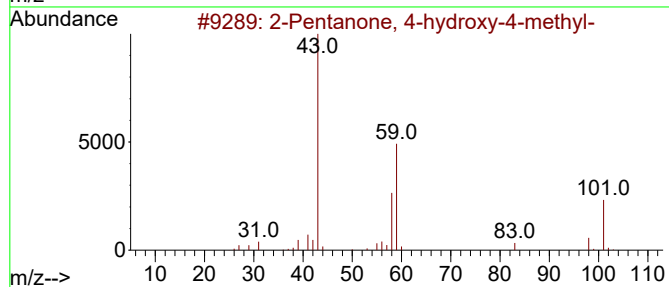
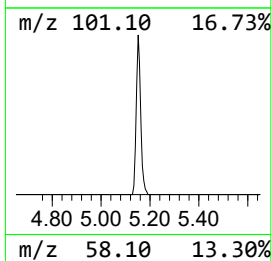
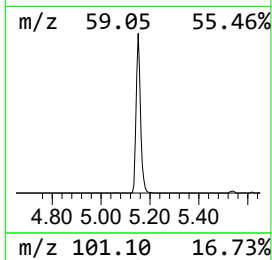
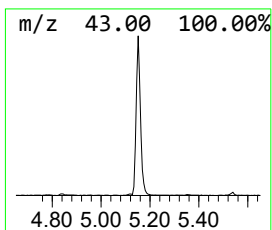
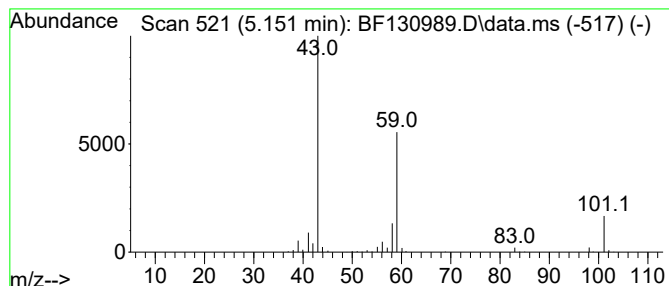
Instrument :
BNA_F
ClientSampleId :
20221104-COMP-03

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.151	10.43 ng	371687	1,4-Dichlorobenzene-d4	6.910	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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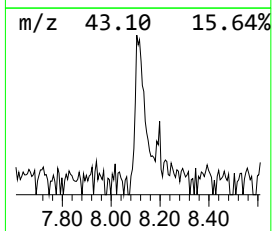
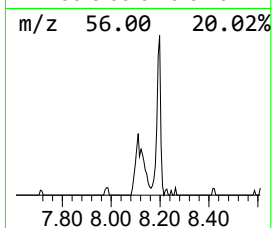
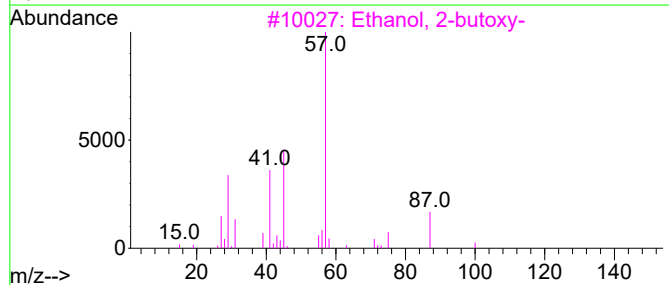
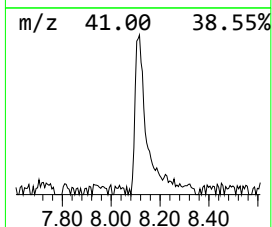
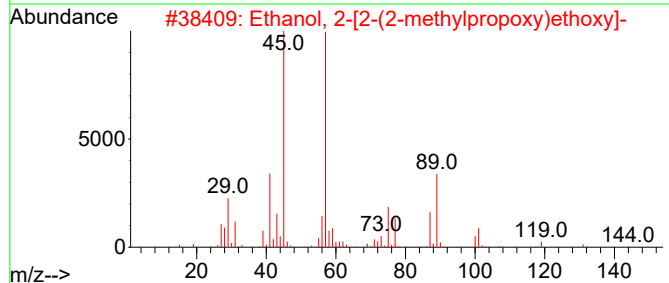
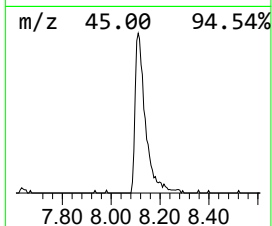
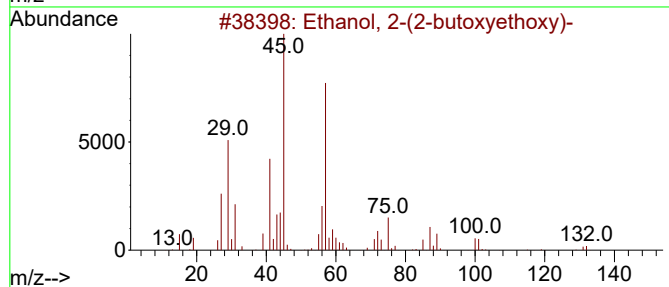
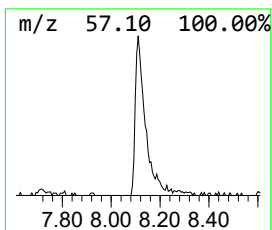
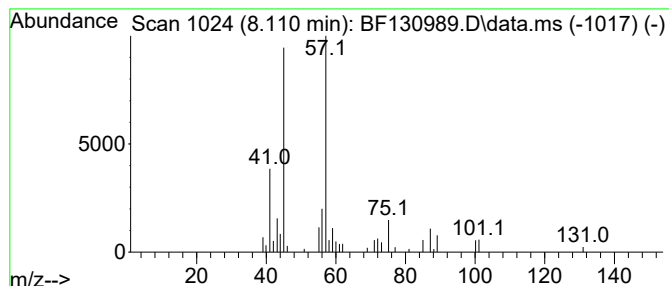
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	3.07 ng	121752	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50



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ALS Vial : 6 Sample Multiplier: 1

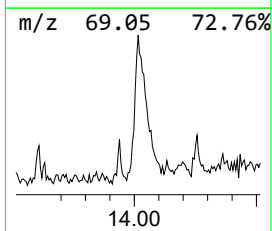
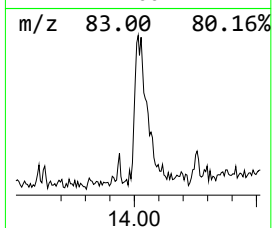
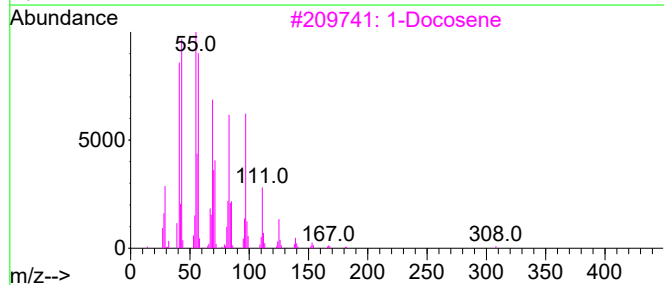
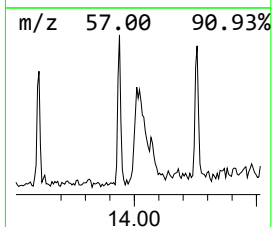
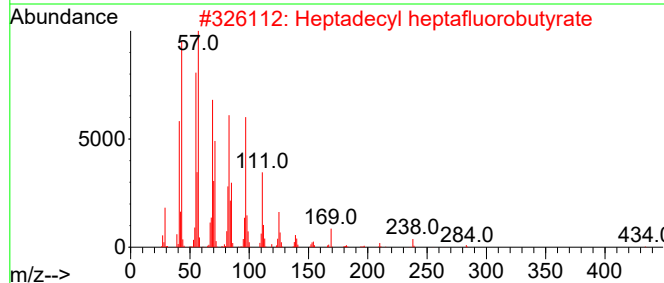
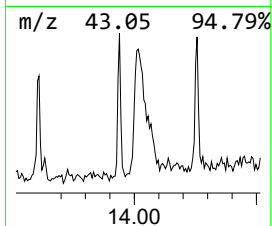
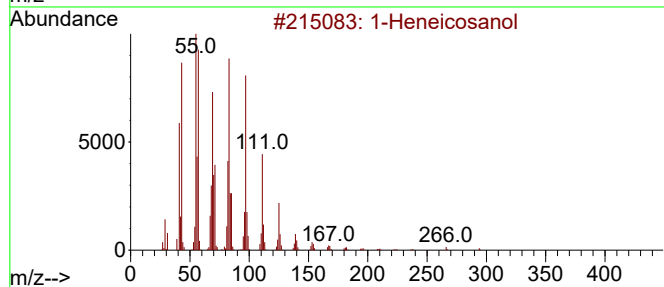
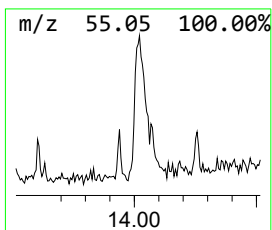
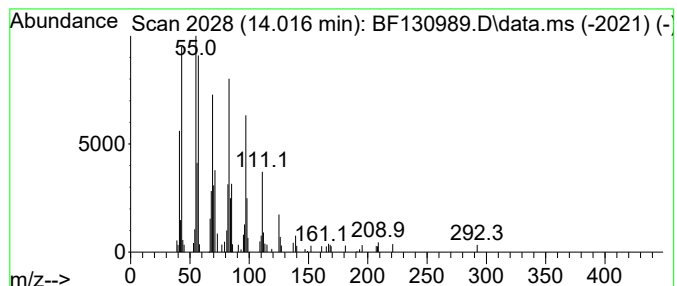
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.015	4.83 ng	194822	Chrysene-d12	14.104	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91



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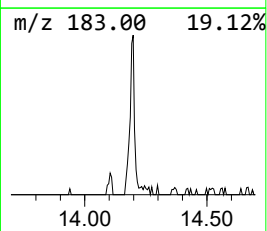
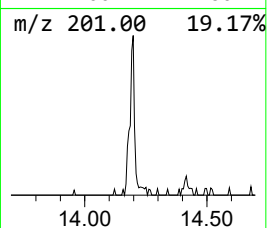
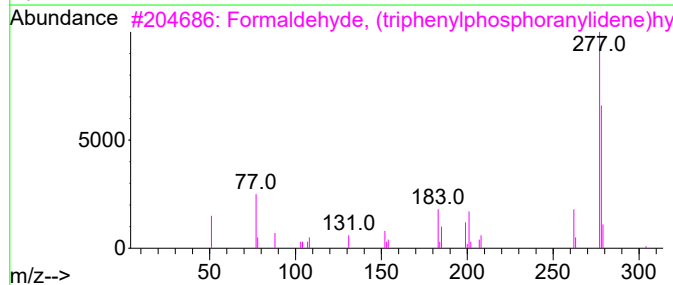
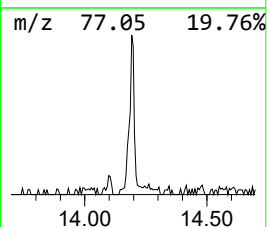
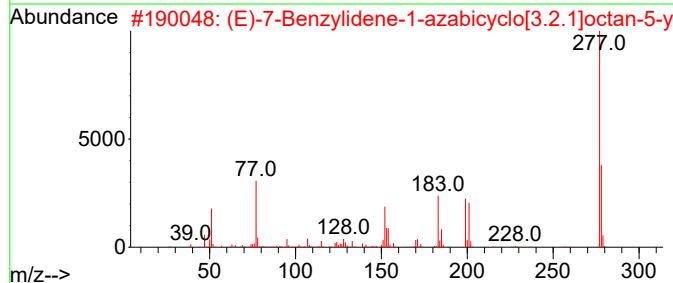
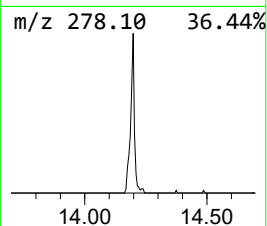
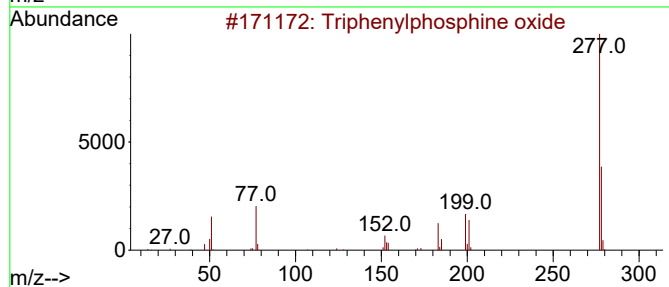
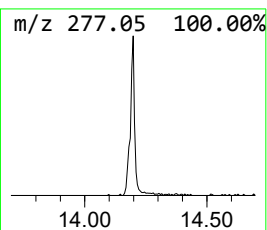
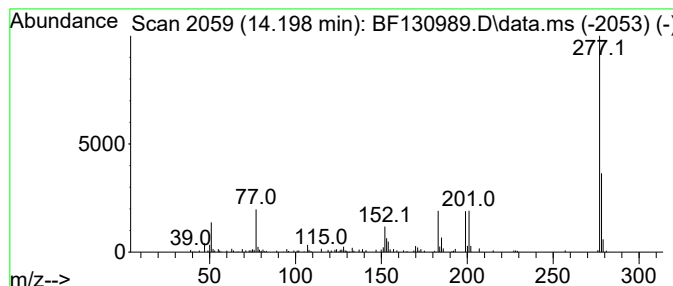
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	2.91 ng	117456	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	58
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	25
5			Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	9



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BNA_F
ClientSampleId :
20221104-COMP-03

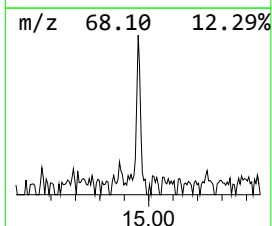
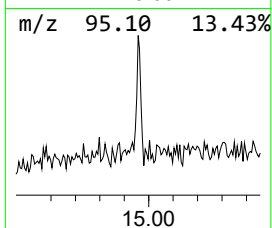
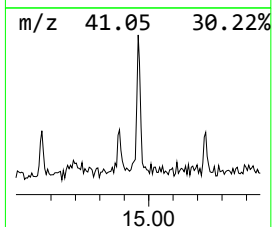
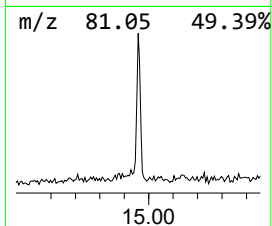
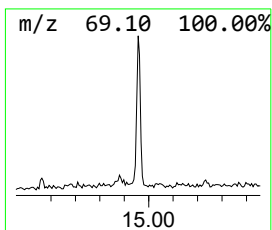
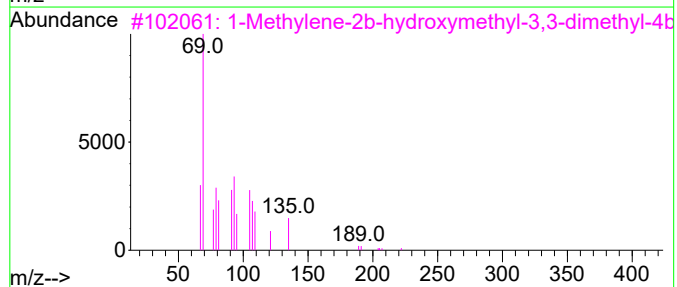
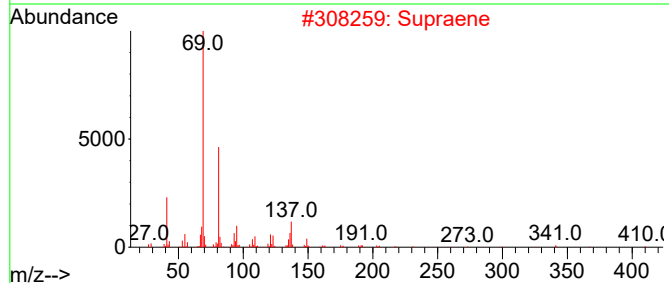
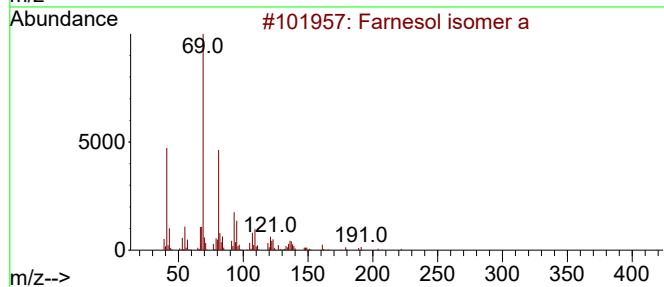
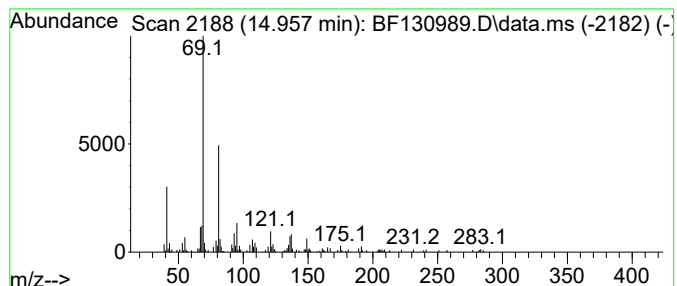
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Farnesol isomer a Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.957	3.55 ng	102558	Perylene-d12	15.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Farnesol isomer a	222	C15H26O	1000108-92-4	83
2			Supraene	410	C30H50	007683-64-9	83
3			1-Methylene-2b-hydroxymethyl-3,3...	222	C15H26O	1000144-10-6	64
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF130989.D
Acq On : 04 Nov 2022 13:25
Operator : CG\JU
Sample : N5272-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221104-COMP-03

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...	2.281	45.1	ng	1606690	1	6.910	712514	20.0
2-Pentanone, 4-...	5.151	10.4	ng	371687	1	6.910	712514	20.0
Ethanol, 2-(2-b...	8.110	3.1	ng	121752	2	8.198	794303	20.0
1-Heneicosanol	14.015	4.8	ng	194822	5	14.104	807217	20.0
Triphenylphosph...	14.198	2.9	ng	117456	5	14.104	807217	20.0
Farnesol isomer a	14.957	3.5	ng	102558	6	15.610	578139	20.0