

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
 Data File : BF130967.D
 Acq On : 03 Nov 2022 19:18
 Operator : CG\JU
 Sample : N5272-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20221109-COMP-08

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: BF130967.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	15	23	28	rVB	1057727	1376343	64.76%	8.292%
2	2.328	37	41	49	rVB	37232	48460	2.28%	0.292%
3	5.140	512	519	526	rVB	225751	277457	13.06%	1.672%
4	5.534	581	586	589	rBV	2086190	1905758	89.67%	11.482%
5	6.539	751	757	767	rBV	1885974	2001493	94.18%	12.058%
6	6.916	817	821	824	rVB	740327	558919	26.30%	3.367%
7	7.481	912	917	920	rBV	1289779	1250254	58.83%	7.532%
8	8.128	1023	1027	1035	rBV	57790	110878	5.22%	0.668%
9	8.198	1035	1039	1043	rVV	841814	723667	34.05%	4.360%
10	9.275	1217	1222	1226	rBV	2191366	2125251	100.00%	12.804%
11	9.963	1334	1339	1342	rBV	936748	824537	38.80%	4.968%
12	10.751	1469	1473	1488	rBV	1213396	1071198	50.40%	6.454%
13	11.451	1589	1592	1596	rBV	892436	795700	37.44%	4.794%
14	11.516	1600	1603	1606	rVB3	35766	30707	1.44%	0.185%
15	11.963	1671	1679	1692	rBV3	196376	304102	14.31%	1.832%
16	12.621	1789	1791	1795	rVB2	25422	25122	1.18%	0.151%
17	12.757	1810	1814	1821	rBV2	75883	111841	5.26%	0.674%
18	13.039	1858	1862	1866	rVB	1731976	1635878	76.97%	9.856%
19	13.721	1974	1978	1990	rVB3	23293	46134	2.17%	0.278%
20	13.939	2012	2015	2020	rVB2	21488	25762	1.21%	0.155%
21	14.051	2030	2034	2039	rBV4	44201	97087	4.57%	0.585%
22	14.098	2039	2042	2046	rVB	531376	501777	23.61%	3.023%
23	14.198	2055	2059	2062	rBV	69956	68705	3.23%	0.414%
24	14.292	2071	2075	2080	rVB2	18855	26787	1.26%	0.161%
25	14.562	2118	2121	2124	rVB3	26960	25685	1.21%	0.155%
26	14.798	2158	2161	2166	rBV3	23860	34440	1.62%	0.207%
27	14.957	2186	2188	2196	rVB	37466	42891	2.02%	0.258%
28	15.233	2232	2235	2239	rVB	27471	32782	1.54%	0.198%
29	15.604	2293	2298	2306	rVB	383988	518706	24.41%	3.125%

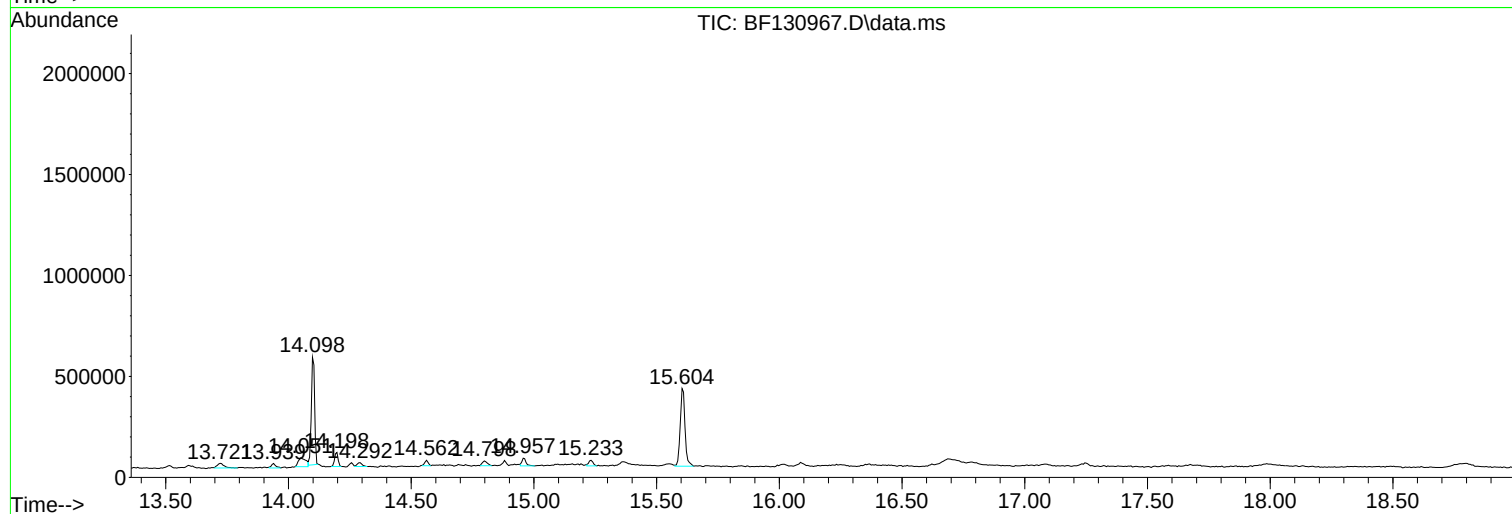
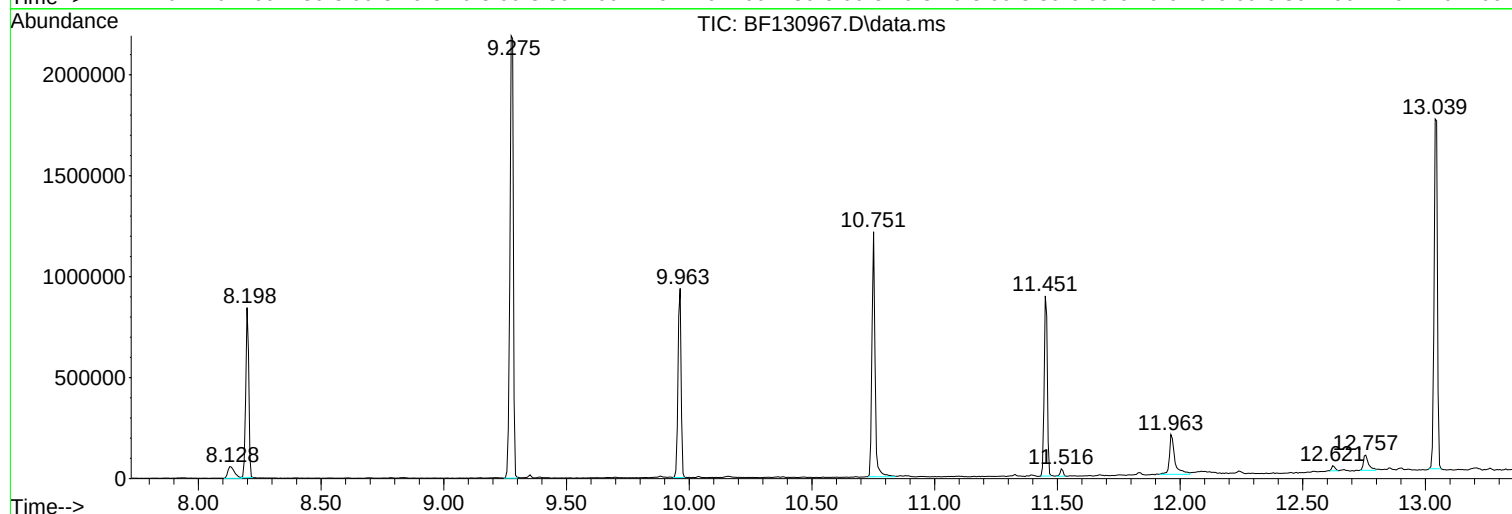
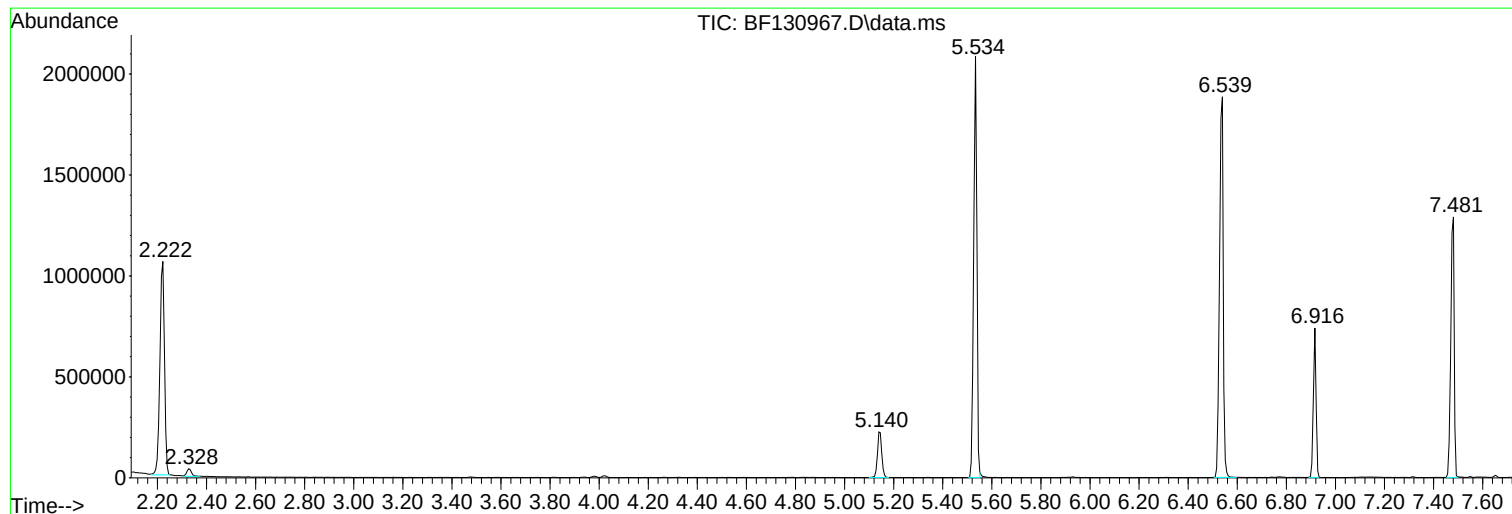
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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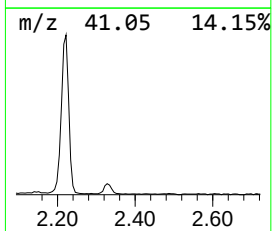
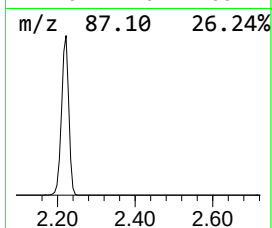
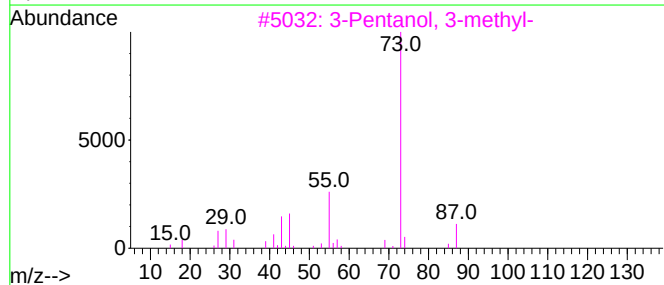
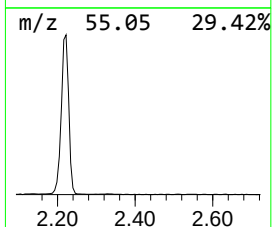
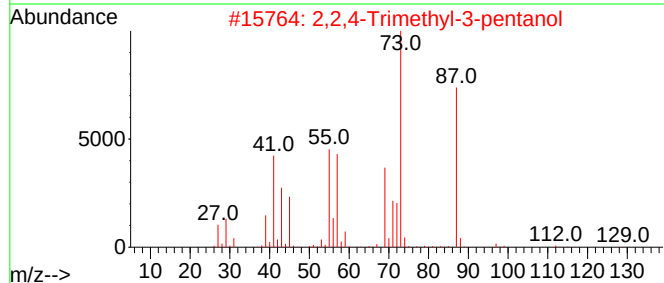
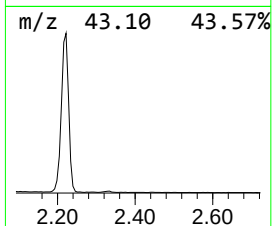
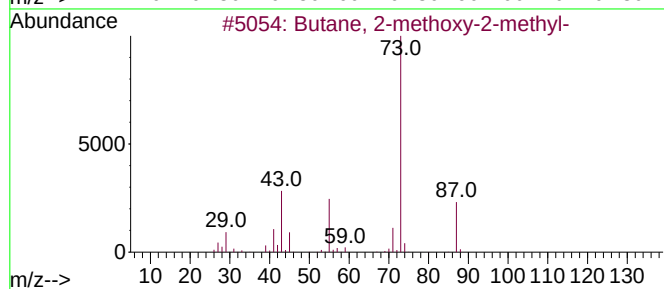
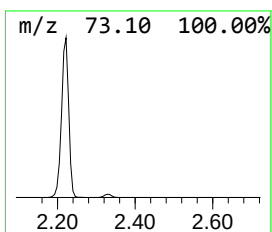
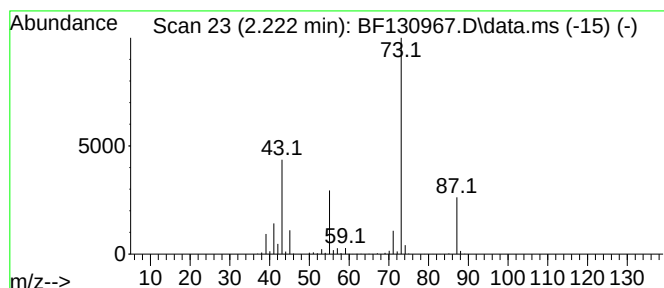
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	49.25 ng	1376340	1,4-Dichlorobenzene-d4	6.916

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	39
3		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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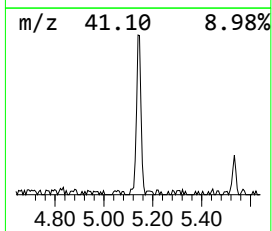
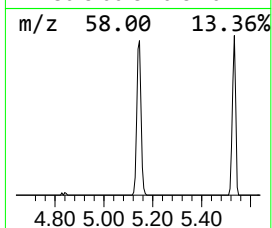
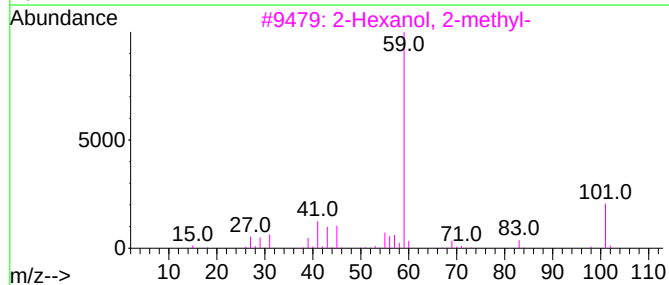
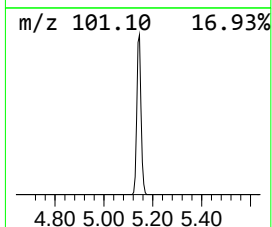
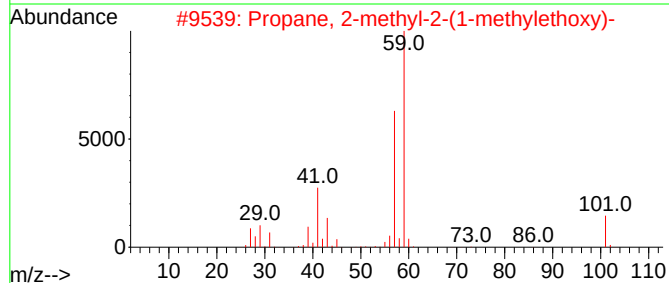
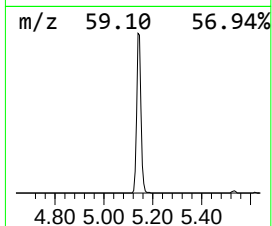
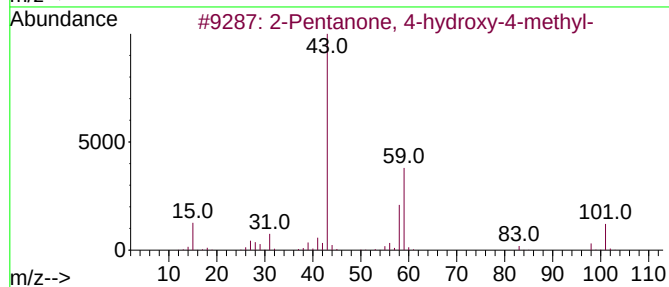
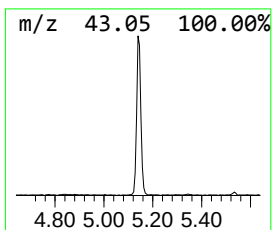
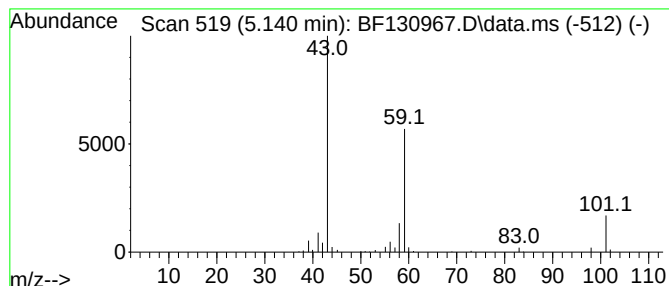
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	9.93 ng	277457	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
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	23



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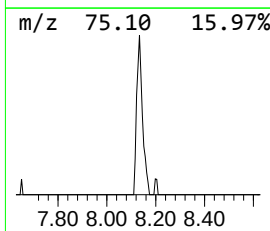
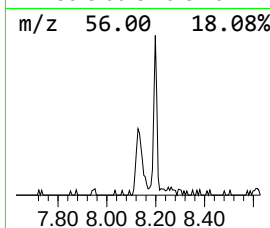
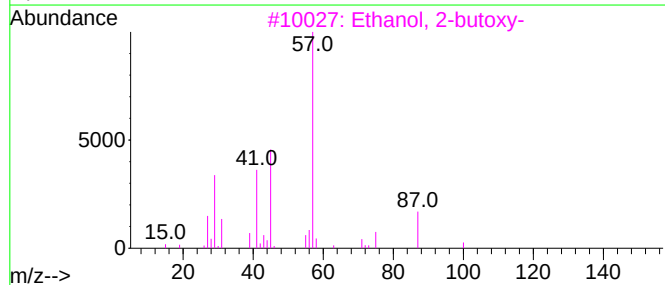
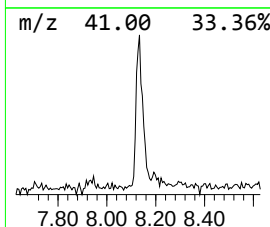
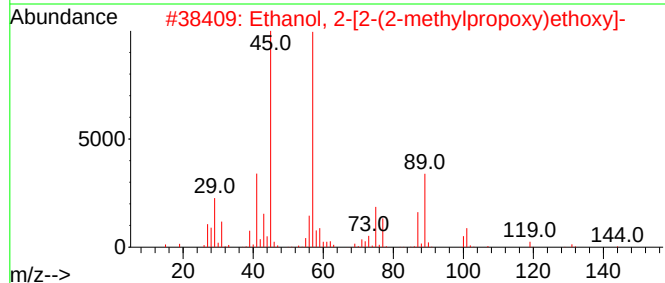
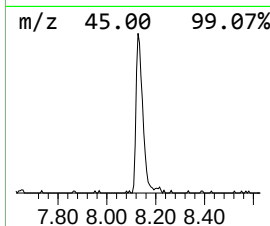
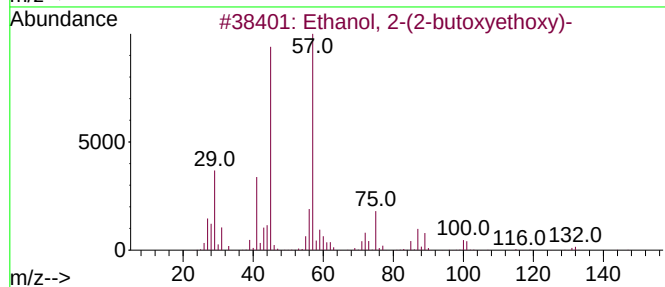
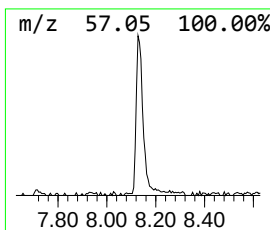
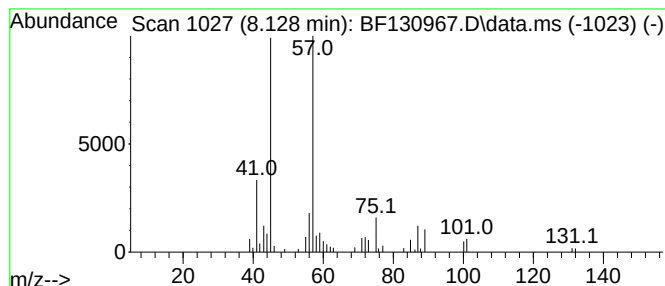
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.128	3.06 ng	110878	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	50
5			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50



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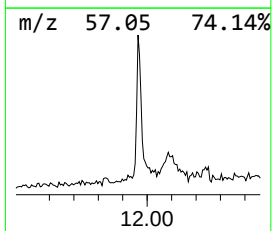
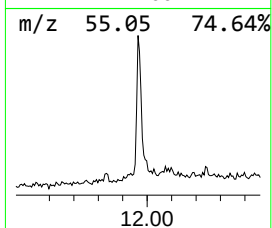
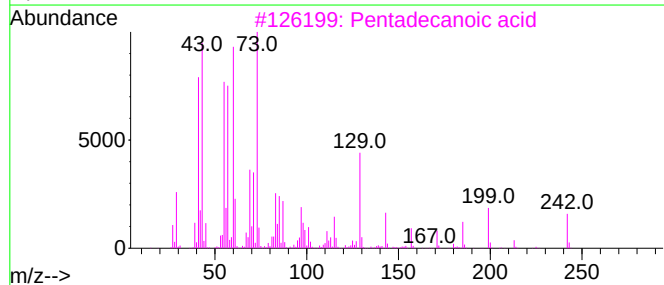
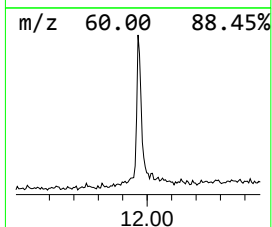
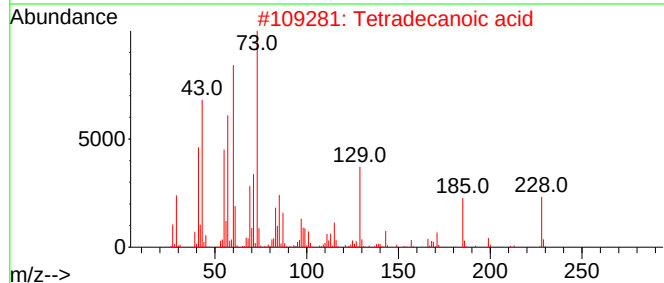
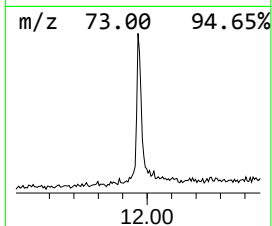
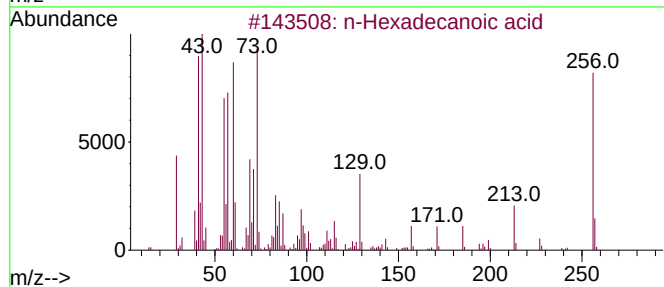
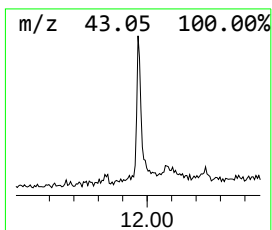
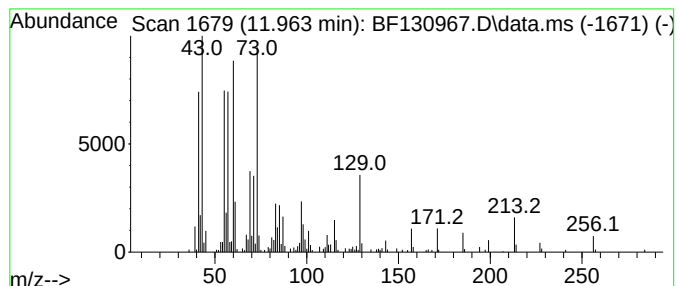
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.963	7.64 ng	304102	Phenanthrene-d10	11.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	70



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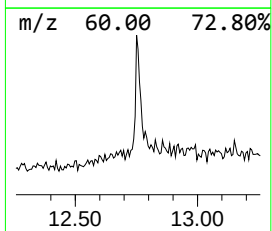
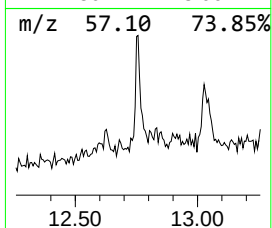
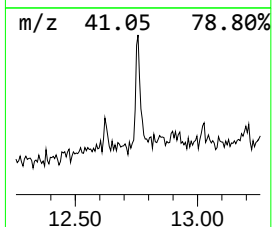
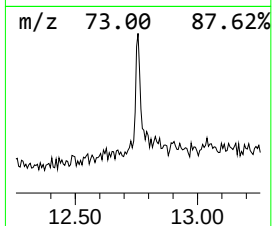
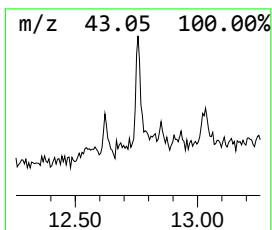
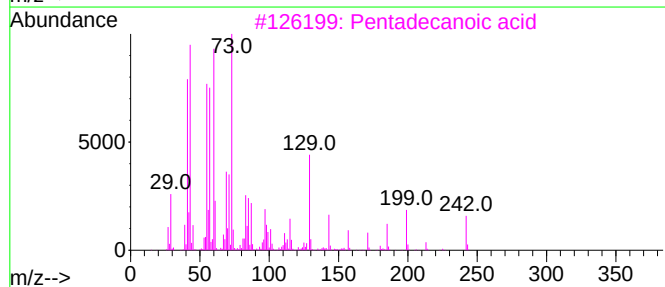
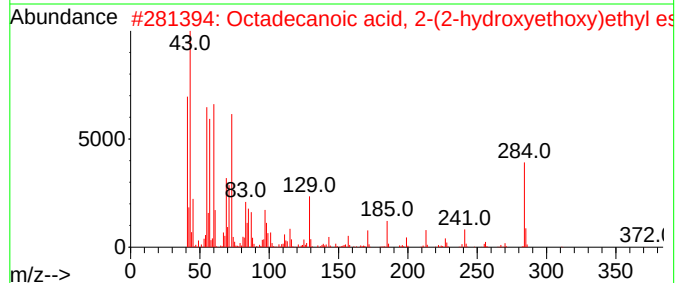
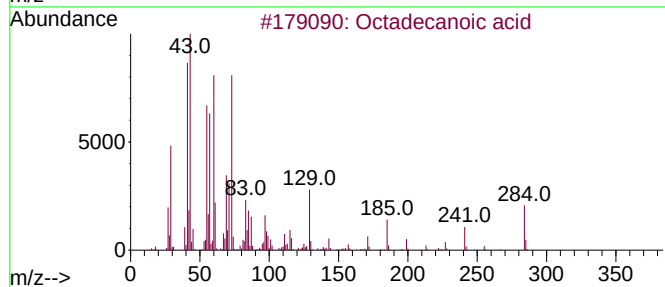
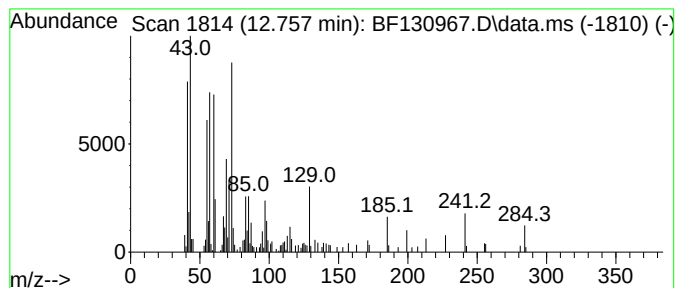
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.757	2.81 ng	111841	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	58



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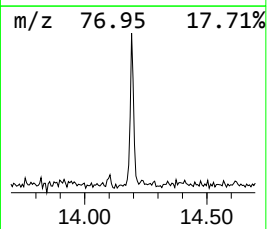
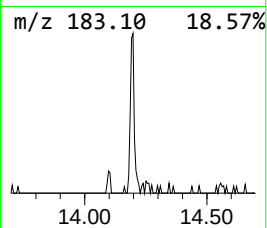
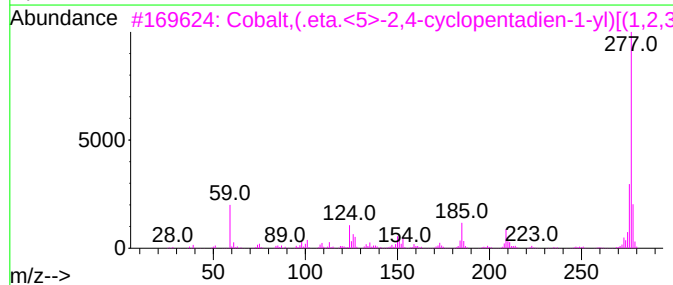
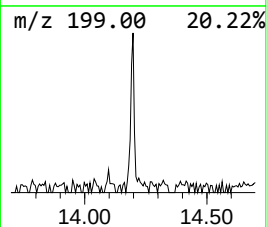
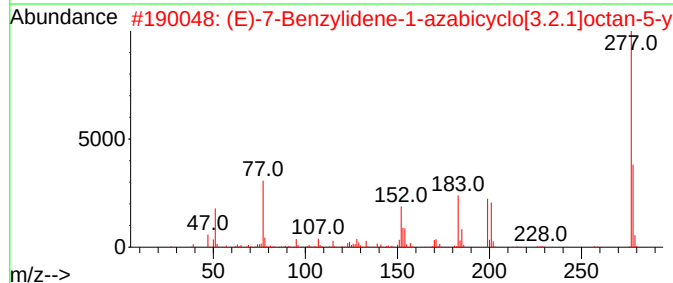
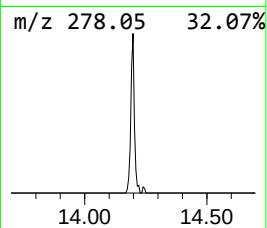
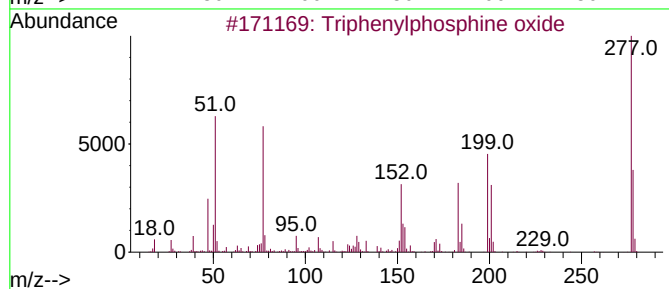
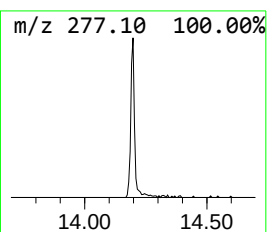
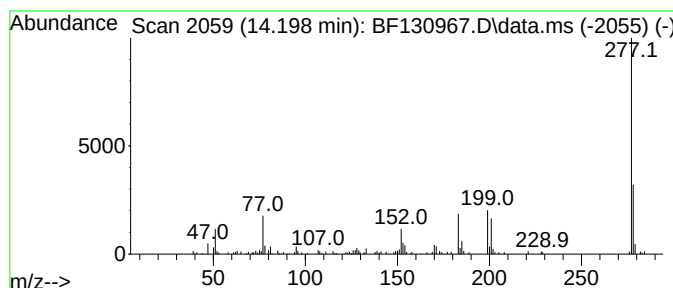
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	2.74 ng	68705	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	47
3			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	37
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130967.D
Acq On : 03 Nov 2022 19:18
Operator : CG\JU
Sample : N5272-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221109-COMP-08

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...	2.222	49.3	ng	1376340	1	6.916	558919	20.0
2-Pentanone, 4-...	5.140	9.9	ng	277457	1	6.916	558919	20.0
Ethanol, 2-(2-b...	8.128	3.1	ng	110878	2	8.198	723667	20.0
n-Hexadecanoic ...	11.963	7.6	ng	304102	4	11.451	795700	20.0
Octadecanoic acid	12.757	2.8	ng	111841	4	11.451	795700	20.0
Triphenylphosph...	14.198	2.7	ng	68705	5	14.098	501777	20.0