

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
 Data File : BF138624.D
 Acq On : 23 Jul 2024 18:04
 Operator : RC/JU
 Sample : P3302-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 285-290

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-BF070924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138624.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	5	13	30	rVB	1247406	1999373	80.20%	9.711%
2	3.399	215	222	236	rBV	74619	170670	6.85%	0.829%
3	5.081	503	508	516	rVB	118374	174143	6.99%	0.846%
4	5.481	570	576	582	rBV	1590877	2108863	84.59%	10.243%
5	6.487	741	747	760	rBV	1601579	2256785	90.53%	10.962%
6	6.681	775	780	792	rVB	62519	85660	3.44%	0.416%
7	6.851	804	809	814	rBV	459294	555496	22.28%	2.698%
8	7.416	898	905	910	rBV	1067132	1448705	58.11%	7.037%
9	7.663	941	947	960	rVB	34994	45708	1.83%	0.222%
10	8.134	1021	1027	1032	rBV	601503	755554	30.31%	3.670%
11	8.351	1058	1064	1068	rBV	22668	29904	1.20%	0.145%
12	8.445	1074	1080	1093	rBV	152406	217559	8.73%	1.057%
13	9.210	1203	1210	1215	rBV	1897729	2492939	100.00%	12.109%
14	9.886	1319	1325	1330	rVB	656708	800249	32.10%	3.887%
15	9.986	1334	1342	1356	rBV	1498502	2419962	97.07%	11.754%
16	10.675	1453	1459	1473	rBV	1012999	1321101	52.99%	6.417%
17	10.792	1474	1479	1488	rVB3	13320	26242	1.05%	0.127%
18	11.369	1572	1577	1584	rBV	537052	679727	27.27%	3.302%
19	11.757	1639	1643	1649	rVB	22685	28068	1.13%	0.136%
20	11.892	1658	1666	1671	rBV	76283	122959	4.93%	0.597%
21	12.463	1752	1763	1773	rVB4	25300	63861	2.56%	0.310%
22	12.810	1818	1822	1826	rBV2	16024	25091	1.01%	0.122%
23	12.951	1841	1846	1851	rBV	1120593	1429396	57.34%	6.943%
24	13.427	1923	1927	1931	rVB	41735	51047	2.05%	0.248%
25	13.857	1994	2000	2015	rBV3	51775	131846	5.29%	0.640%
26	14.004	2017	2025	2036	rVB	335976	458297	18.38%	2.226%
27	14.468	2100	2104	2107	rBV	17966	25215	1.01%	0.122%
28	14.845	2164	2168	2176	rVB	26834	39886	1.60%	0.194%
29	15.039	2197	2201	2208	rBV	17444	34723	1.39%	0.169%
30	15.110	2208	2213	2217	rVB	38828	54083	2.17%	0.263%
31	15.468	2268	2274	2285	rVB	266765	418009	16.77%	2.030%
32	15.915	2345	2350	2357	rBV	48004	83906	3.37%	0.408%
33	17.009	2532	2536	2546	rVB3	14783	32909	1.32%	0.160%

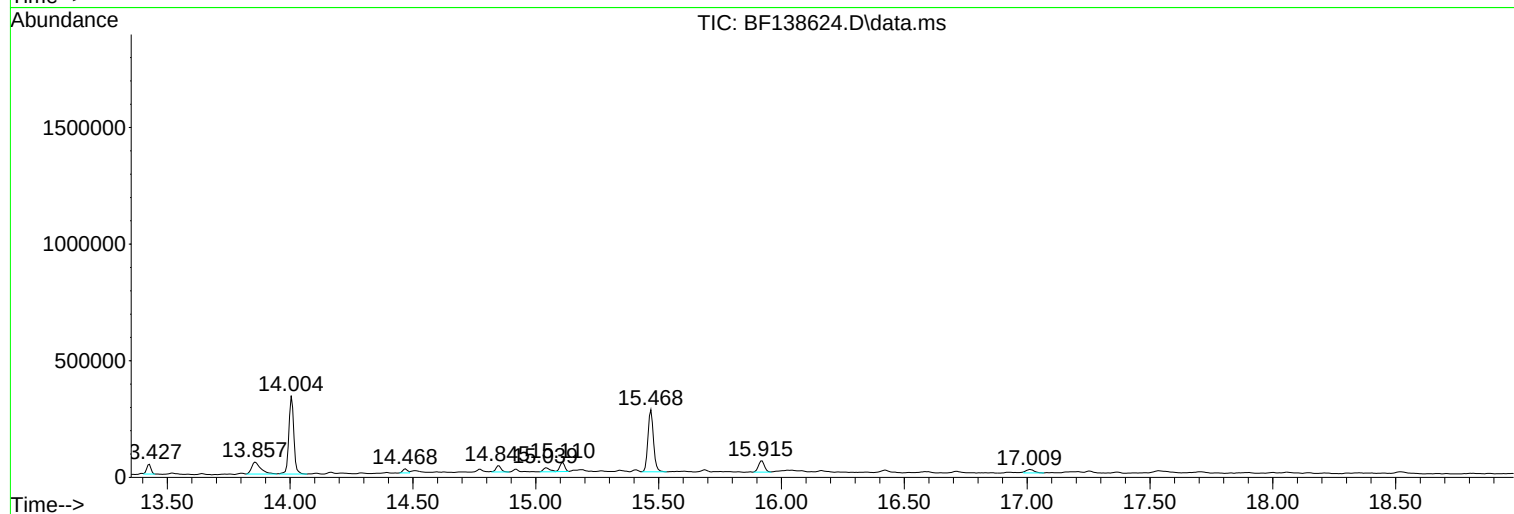
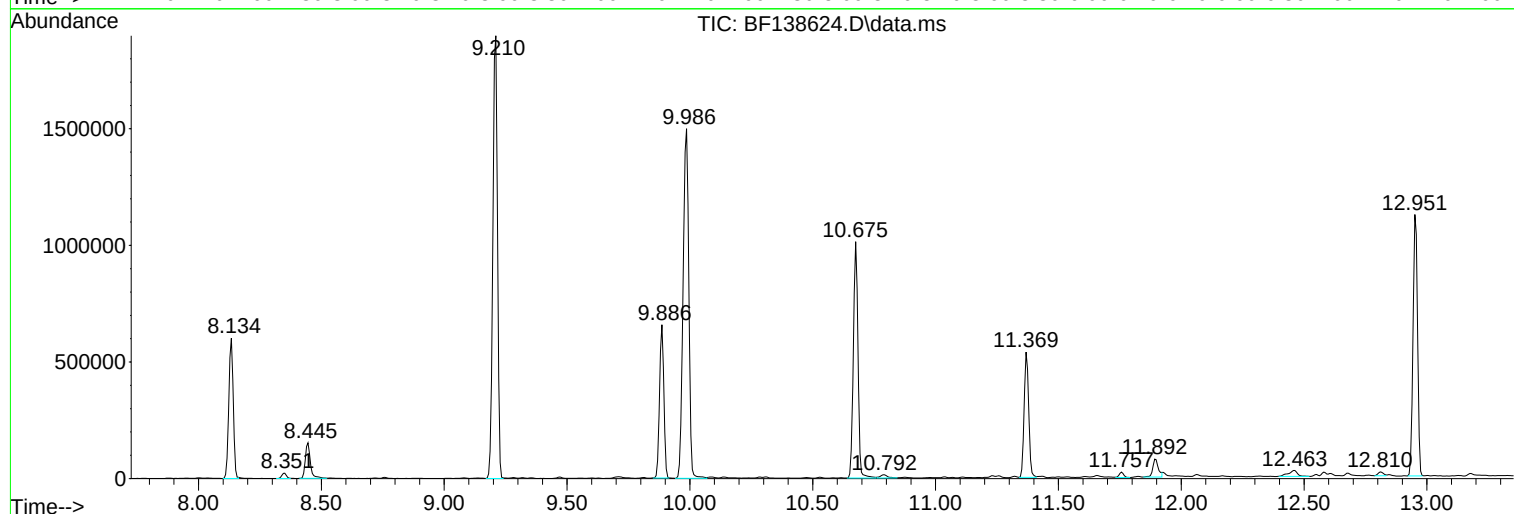
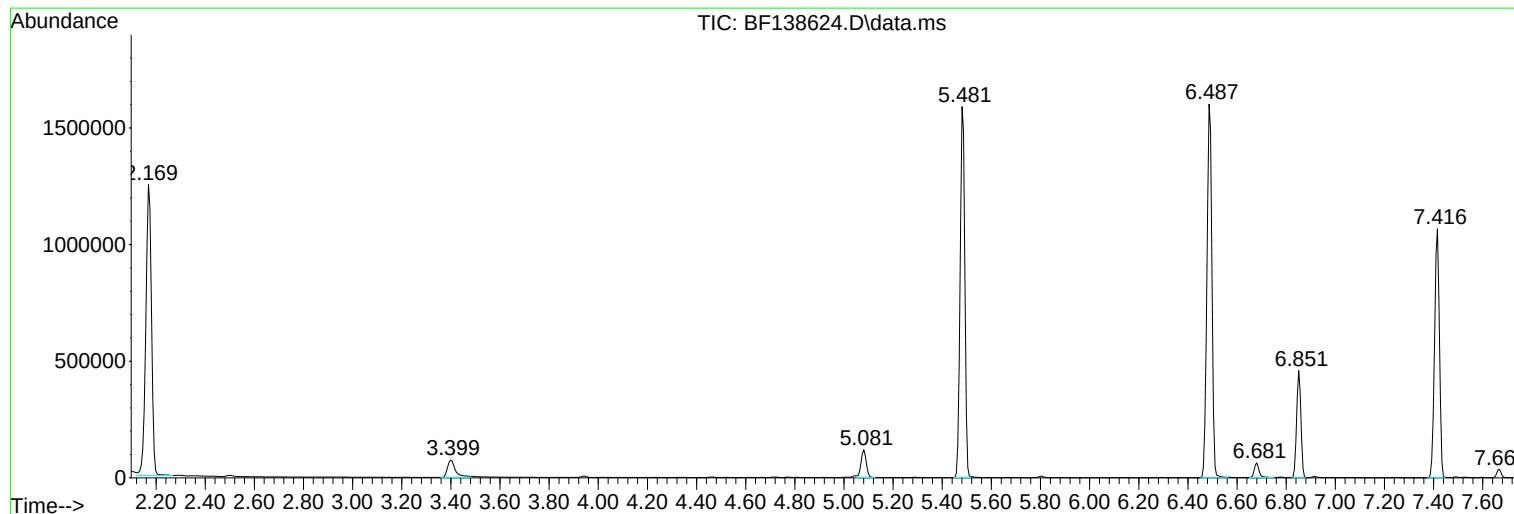
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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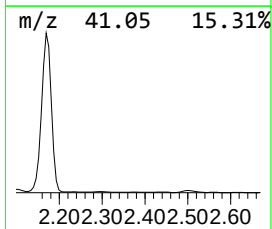
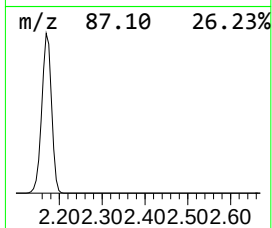
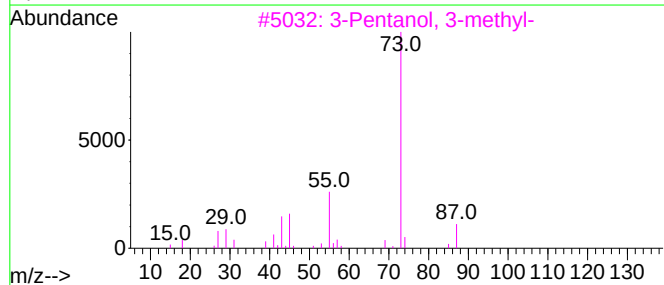
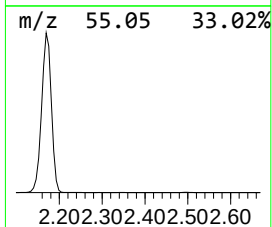
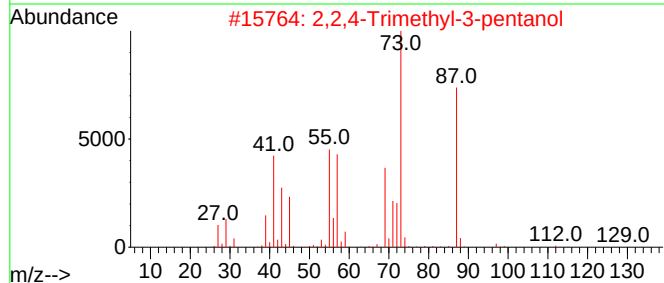
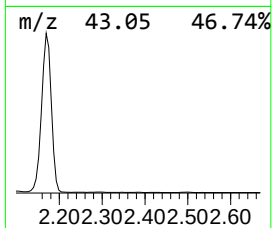
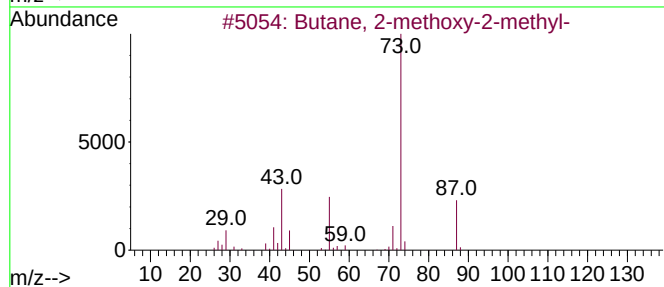
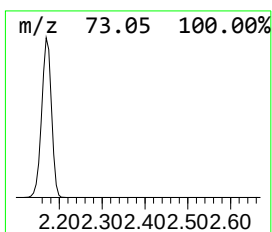
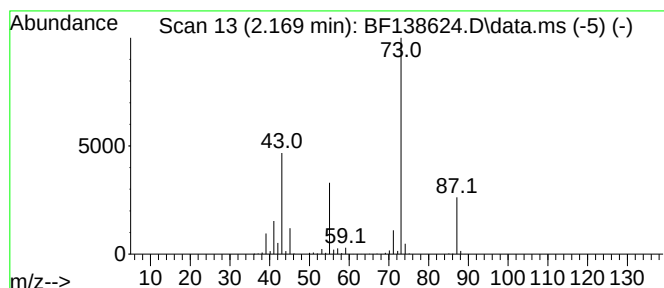
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	71.99 ng	1999370	1,4-Dichlorobenzene-d4	6.851

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			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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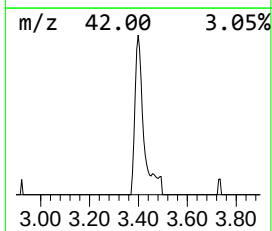
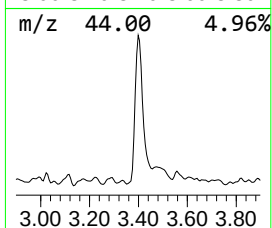
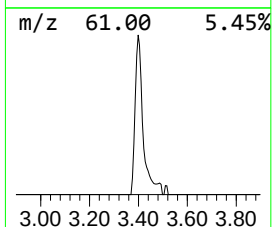
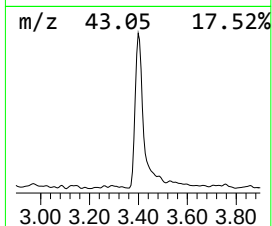
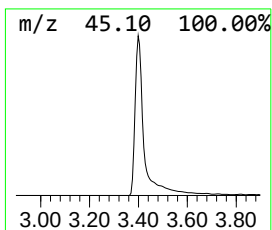
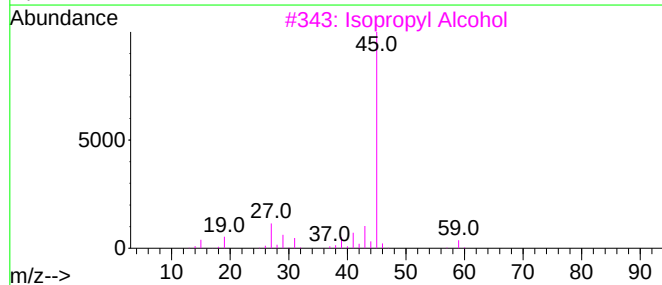
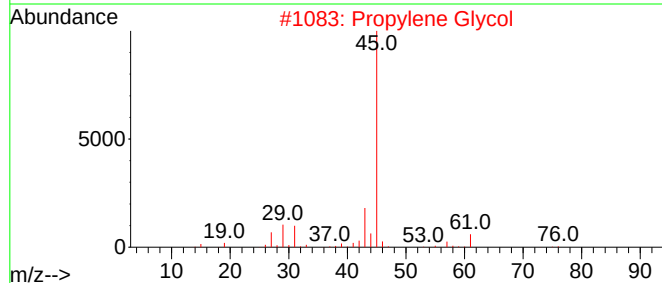
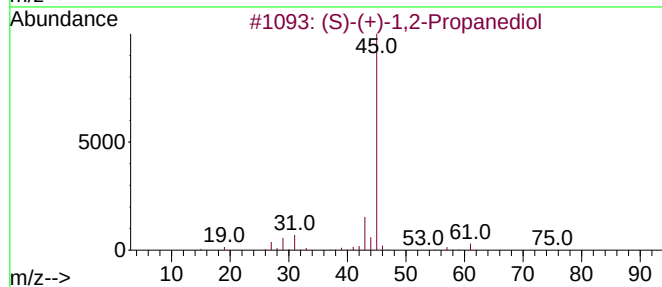
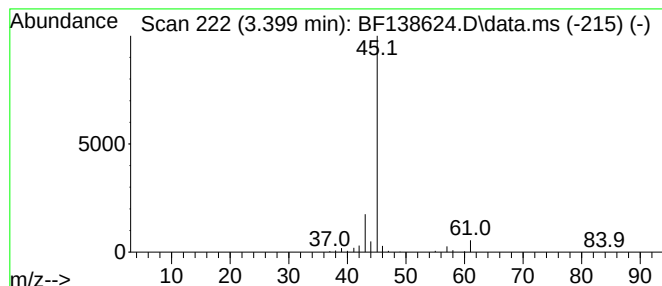
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown3.399 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	6.14 ng	170670	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	43
2	Propylene Glycol			76	C3H8O2	000057-55-6	43
3	Isopropyl Alcohol			60	C3H8O	000067-63-0	9
4	Methyltartronic acid			134	C4H6O5	000595-98-2	9
5	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	9



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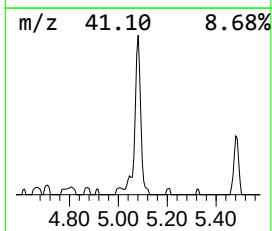
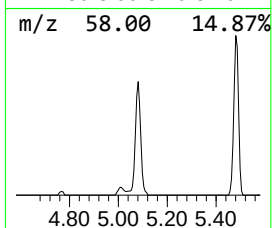
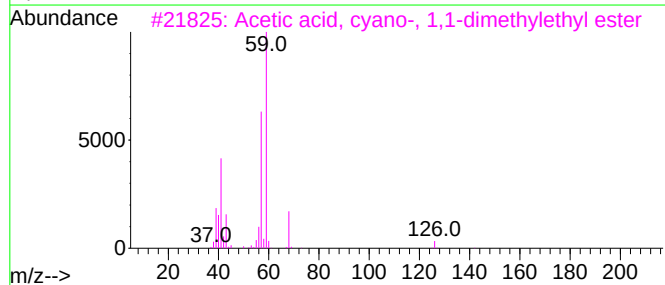
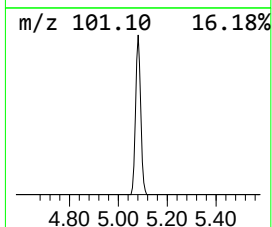
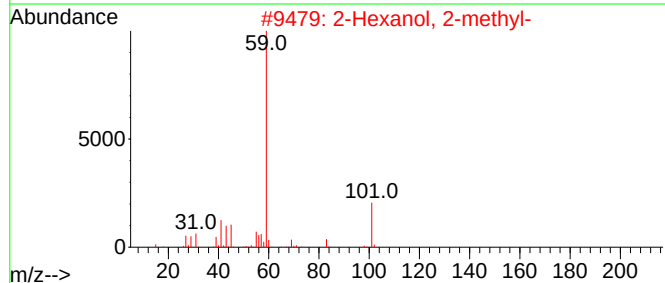
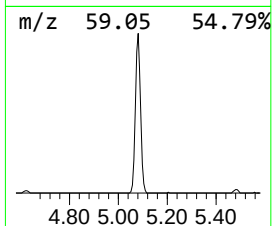
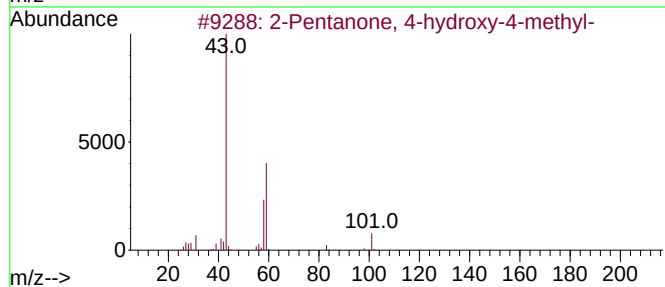
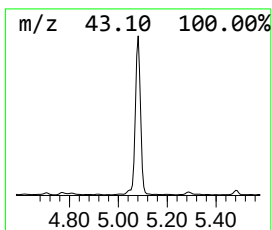
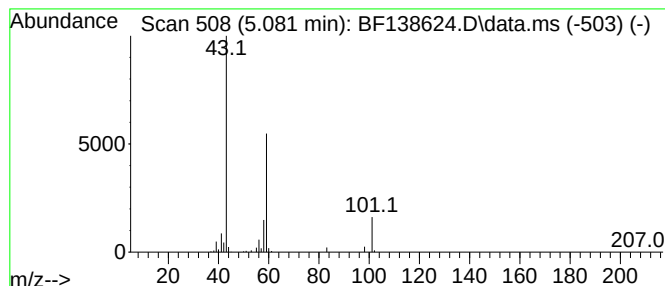
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	6.27 ng	174143	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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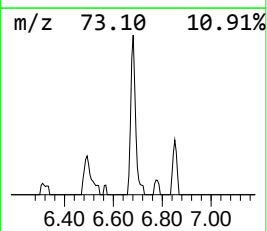
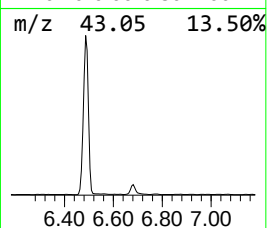
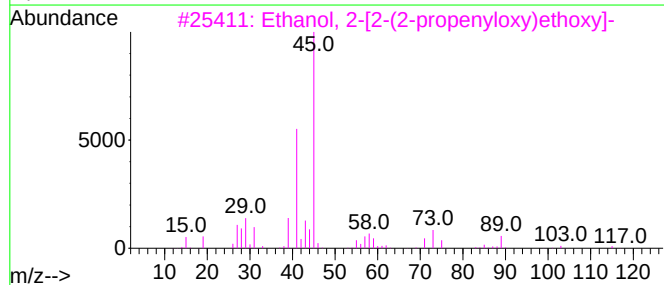
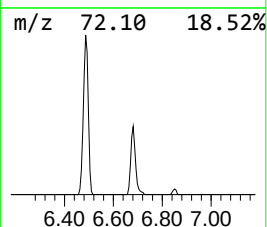
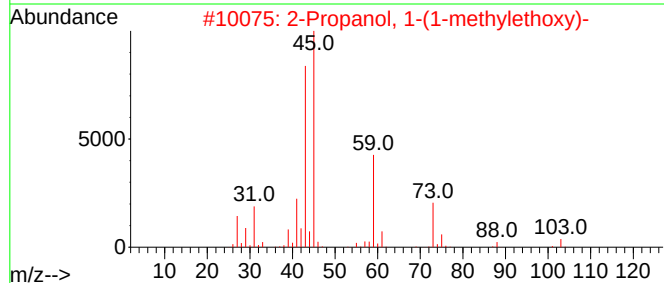
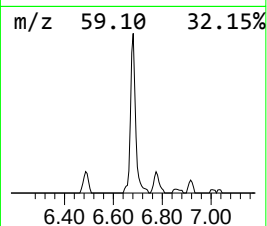
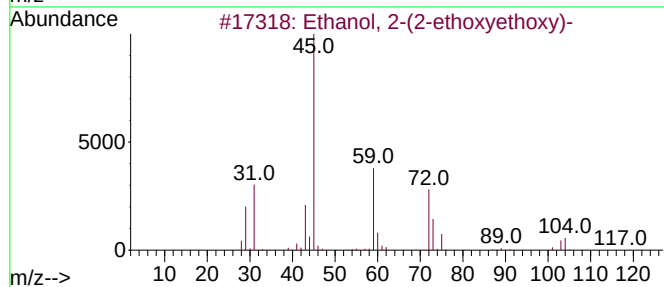
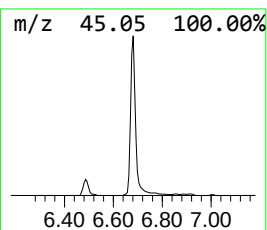
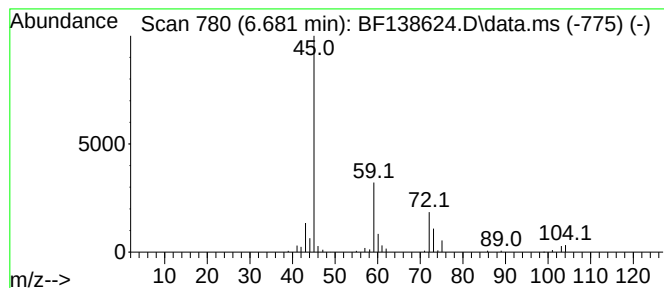
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Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	3.08 ng	85660	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
3			Ethanol, 2-[2-(2-propenyloxy)eth...]	146	C7H14O3	015075-50-0	38
4			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	38
5			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	38



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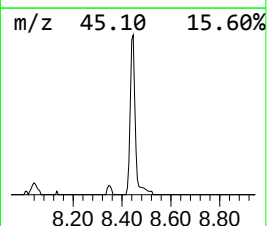
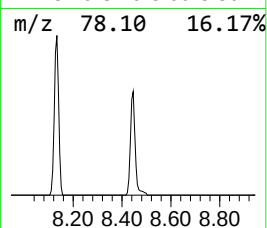
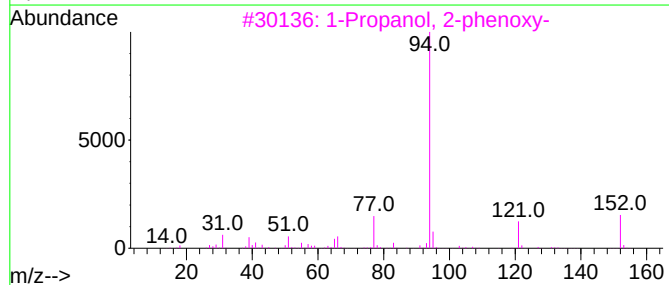
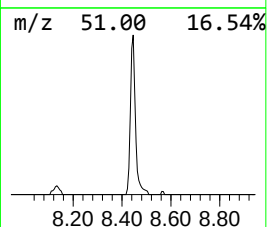
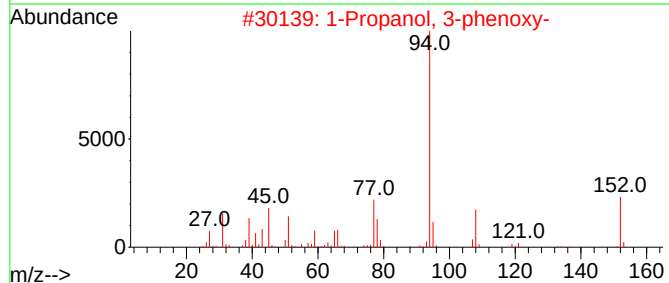
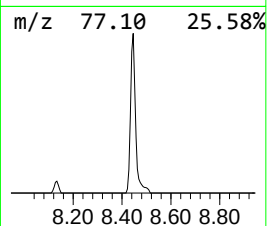
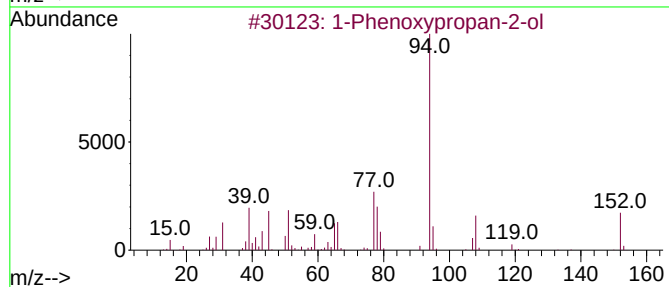
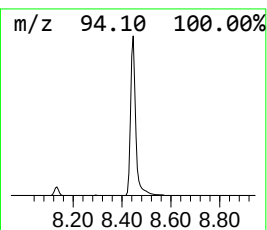
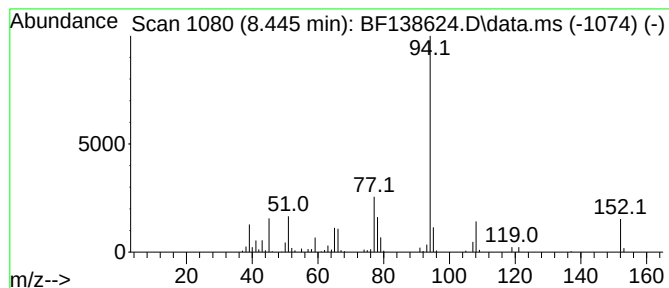
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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	5.76 ng	217559	Naphthalene-d8	8.134

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5		tert-Butyl phenyl carbonate	194	C11H14O3	006627-89-0	53



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285-290

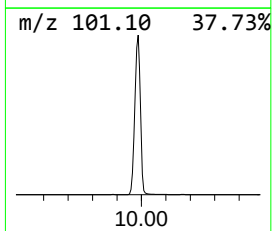
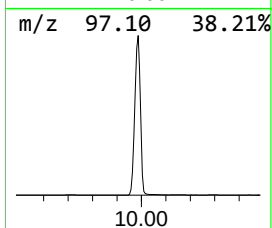
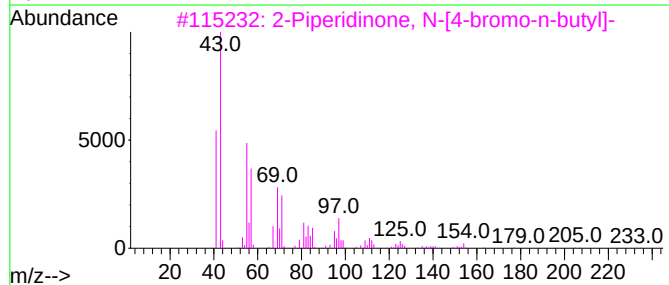
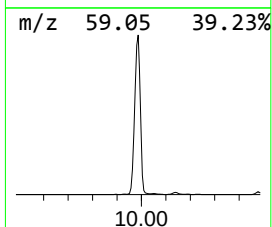
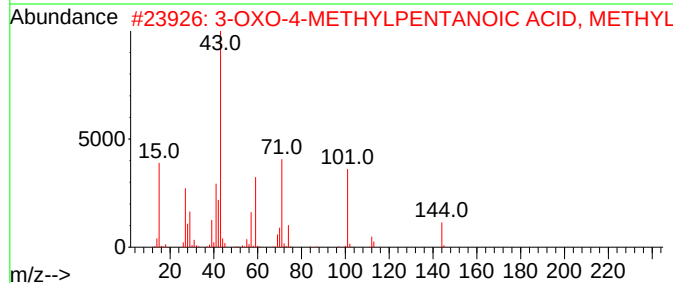
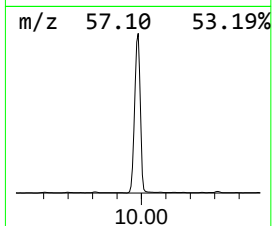
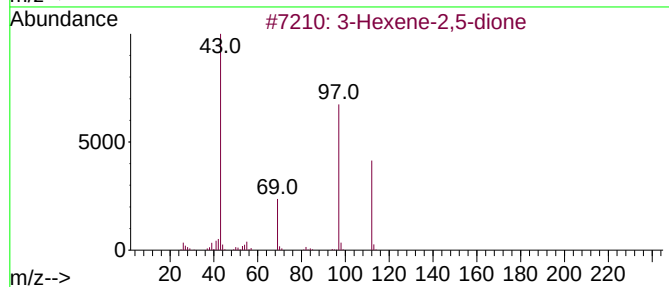
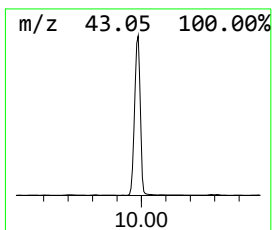
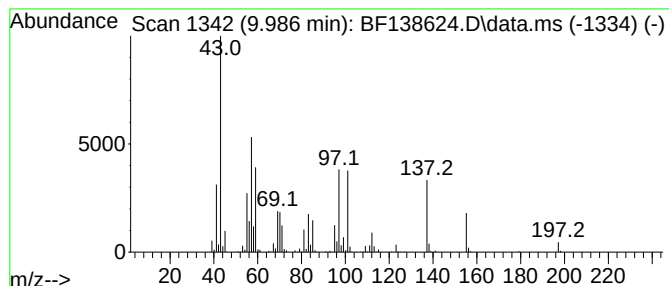
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.986 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	60.48 ng	2419960	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexene-2,5-dione			112	C6H8O2	004436-75-3	18
2	3-OXO-4-METHYLPENTANOIC ACID, ME...			144	C7H12O3	042558-54-3	16
3	2-Piperidinone, N-[4-bromo-n-but...			233	C9H16BrNO	195194-80-0	14
4	Acetic acid, 1,1-dimethylethyl e...			116	C6H12O2	000540-88-5	12
5	2-Hexanone, 4-methyl-			114	C7H14O	000105-42-0	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
Data File : BF138624.D
Acq On : 23 Jul 2024 18:04
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
285-290

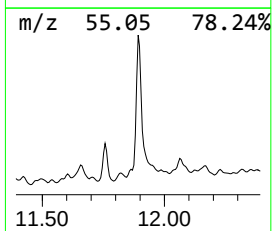
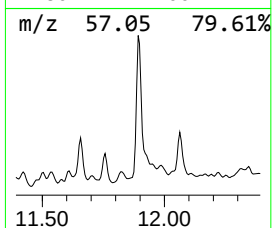
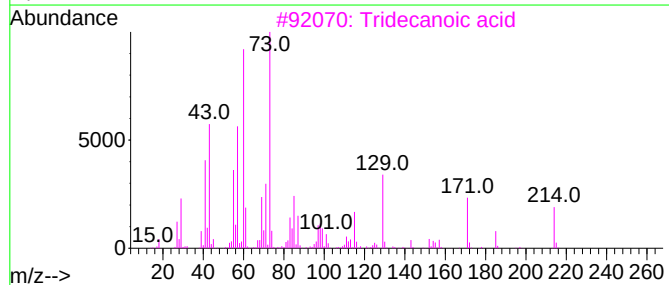
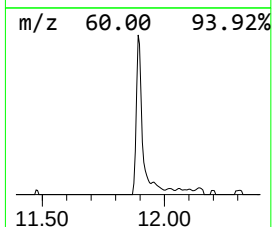
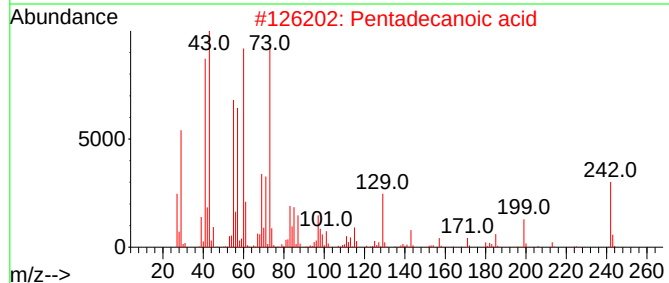
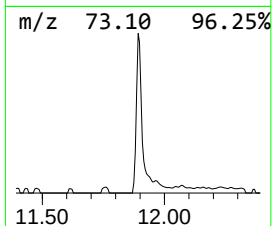
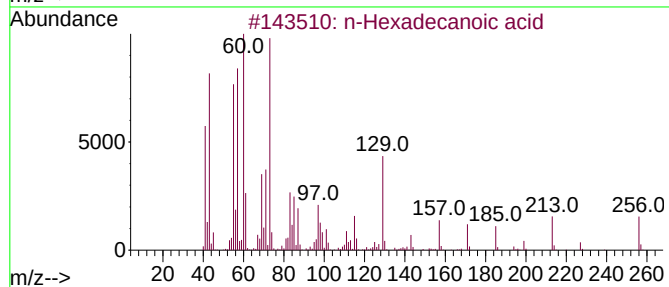
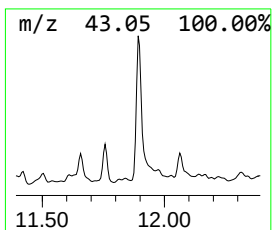
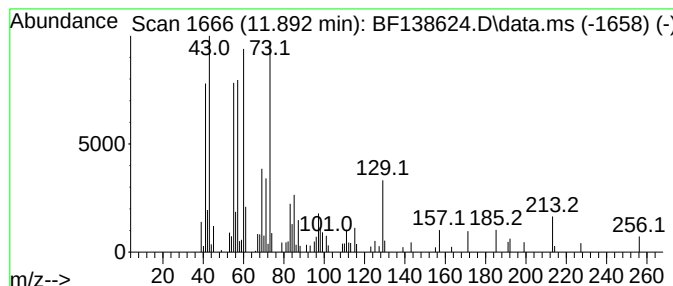
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.62 ng	122959	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
Data File : BF138624.D
Acq On : 23 Jul 2024 18:04
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
285-290

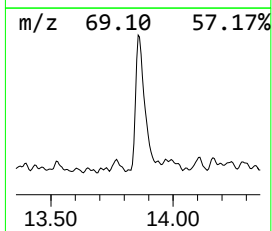
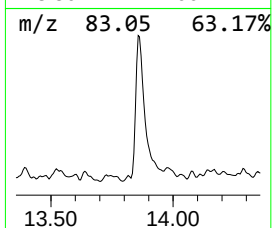
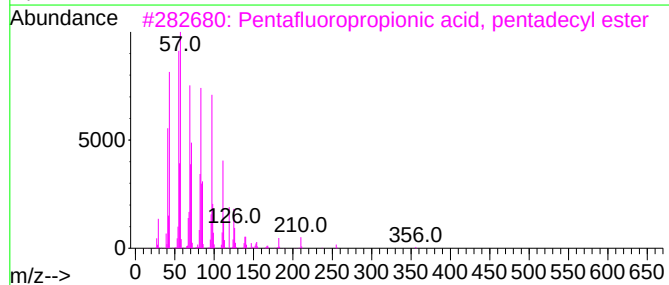
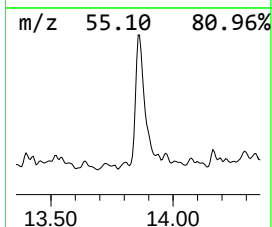
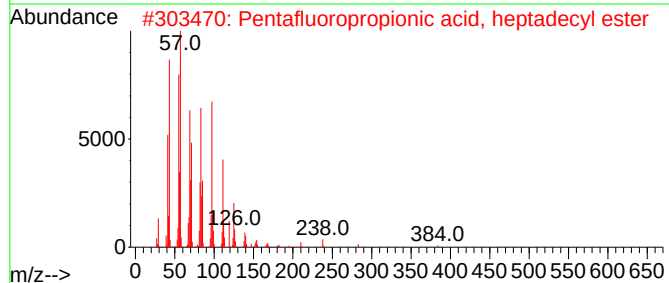
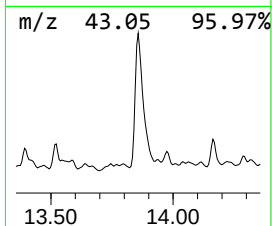
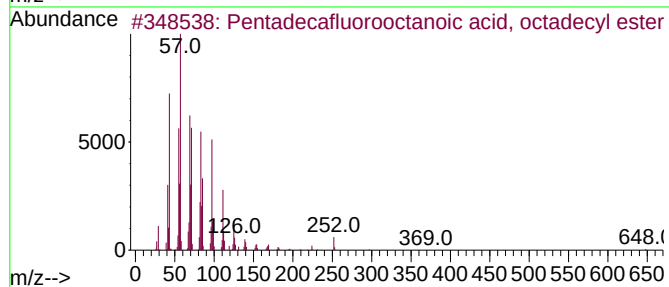
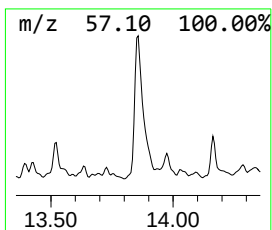
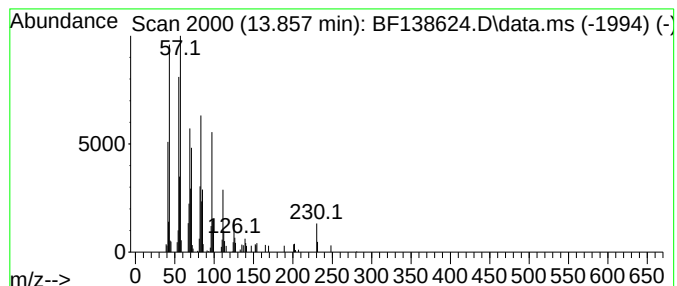
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	5.75 ng	131846	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
Data File : BF138624.D
Acq On : 23 Jul 2024 18:04
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
285-290

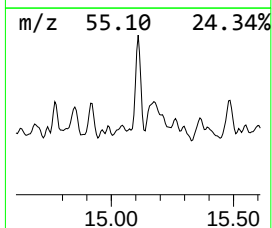
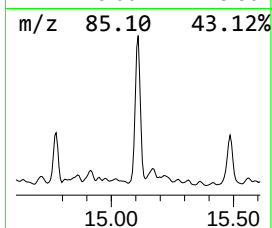
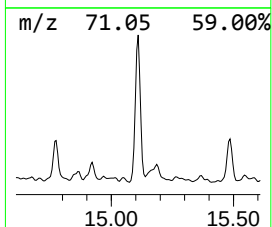
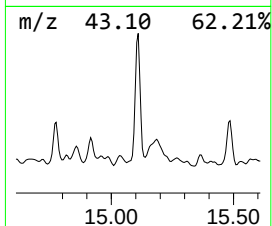
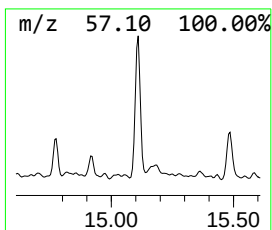
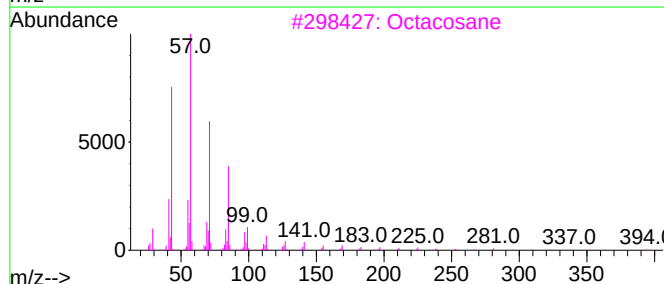
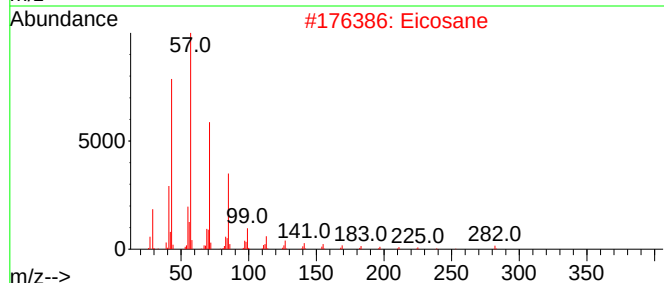
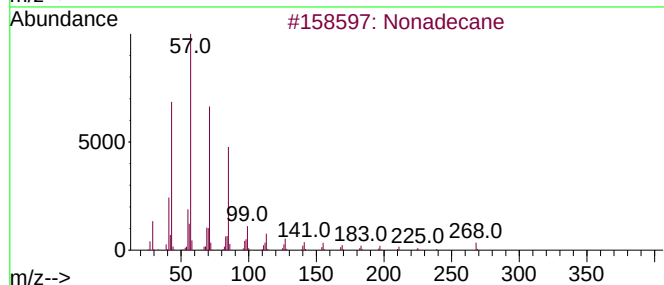
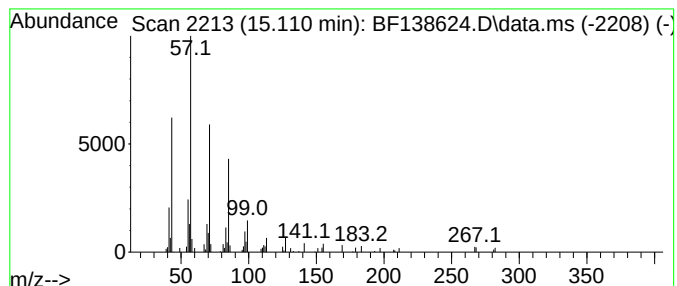
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	2.59 ng	54083	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	96
2			Eicosane	282	C20H42	000112-95-8	93
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
Data File : BF138624.D
Acq On : 23 Jul 2024 18:04
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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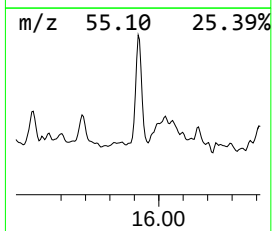
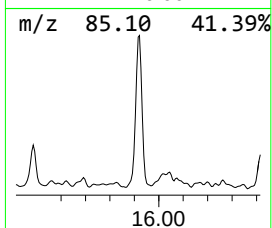
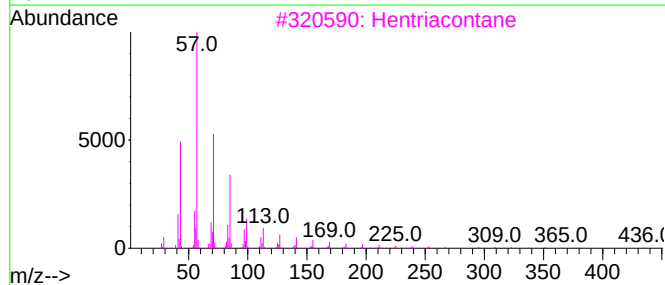
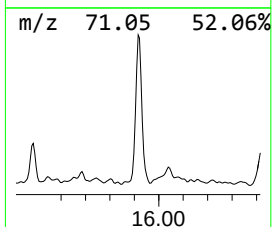
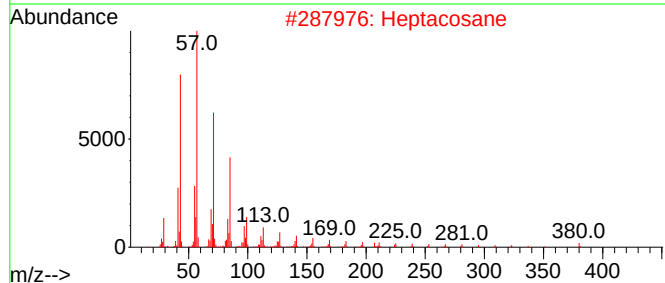
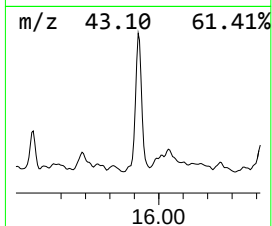
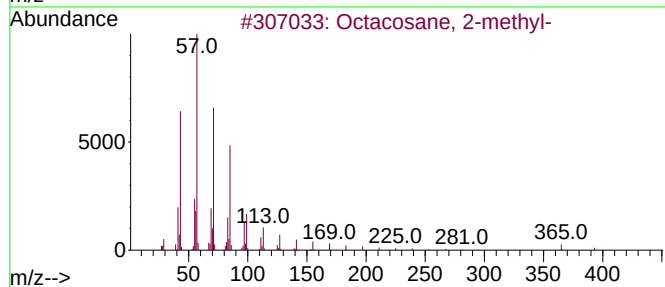
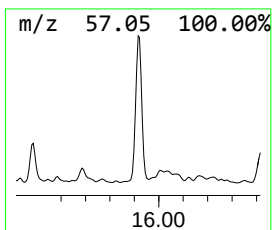
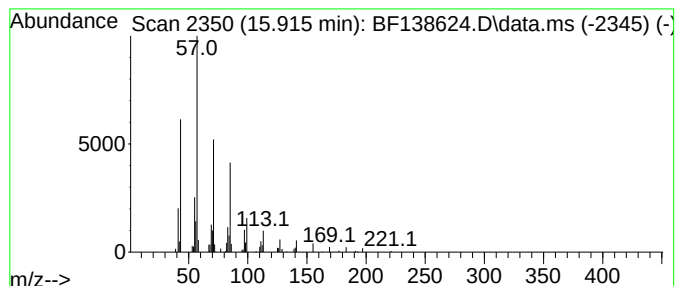
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	4.01 ng	83906	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Hentriacontane	437	C31H64	000630-04-6	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
Data File : BF138624.D
Acq On : 23 Jul 2024 18:04
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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
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unknown3.399	3.399	6.1	ng	170670	1	6.851	555496	20.0
2-Pentanone, 4-...	5.081	6.3	ng	174143	1	6.851	555496	20.0
Ethanol, 2-(2-e...	6.681	3.1	ng	85660	1	6.851	555496	20.0
1-Phenoxypropan...	8.445	5.8	ng	217559	2	8.134	755554	20.0
unknown9.986	9.986	60.5	ng	2419960	3	9.886	800249	20.0
n-Hexadecanoic ...	11.892	3.6	ng	122959	4	11.369	679727	20.0
Pentadecafluoro...	13.857	5.8	ng	131846	5	14.004	458297	20.0
Nonadecane	15.110	2.6	ng	54083	6	15.468	418009	20.0
Octacosane, 2-m...	15.915	4.0	ng	83906	6	15.468	418009	20.0