

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
 Data File : BF138534.D
 Acq On : 11 Jul 2024 20:52
 Operator : CG\JU
 Sample : P3208-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 352

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: BF138534.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	13	19	rVB	1604735	2105453	89.88%	9.847%
2	3.387	219	221	230	rBV	50600	96931	4.14%	0.453%
3	5.087	507	510	516	rVB	141533	163392	6.97%	0.764%
4	5.492	574	579	582	rBV	2354570	2105603	89.88%	9.848%
5	6.498	745	750	753	rBV	2280294	2123388	90.64%	9.931%
6	6.687	779	782	788	rBV	39148	37512	1.60%	0.175%
7	6.863	808	812	815	rBV	787165	598080	25.53%	2.797%
8	7.428	902	908	911	rBV	1461062	1429094	61.00%	6.684%
9	7.675	947	950	955	rVB	52585	40773	1.74%	0.191%
10	8.145	1025	1030	1032	rBV	875242	783824	33.46%	3.666%
11	8.163	1032	1033	1037	rVB	40333	25101	1.07%	0.117%
12	8.451	1079	1082	1095	rVB	116609	128460	5.48%	0.601%
13	9.216	1207	1212	1215	rBV	2514692	2342619	100.00%	10.956%
14	9.898	1324	1328	1331	rBV	917432	768318	32.80%	3.593%
15	9.998	1339	1345	1353	rBV	1048418	1393428	59.48%	6.517%
16	10.680	1457	1461	1465	rBV	1137028	1086865	46.40%	5.083%
17	10.804	1478	1482	1489	rVB4	19416	32265	1.38%	0.151%
18	11.380	1576	1580	1582	rBV	776897	638255	27.25%	2.985%
19	11.404	1582	1584	1587	rVV	151296	119349	5.09%	0.558%
20	11.457	1590	1593	1595	rVB	31656	30393	1.30%	0.142%
21	11.880	1662	1665	1667	rBV	29095	30573	1.31%	0.143%
22	11.904	1667	1669	1677	rVV3	232755	229462	9.80%	1.073%
23	11.992	1681	1684	1686	rBV2	39939	41561	1.77%	0.194%
24	12.074	1696	1698	1701	rBV2	20060	24420	1.04%	0.114%
25	12.227	1722	1724	1727	rBV2	22346	27649	1.18%	0.129%
26	12.357	1743	1746	1748	rBV2	41660	40893	1.75%	0.191%
27	12.433	1756	1759	1762	rBV4	38983	51476	2.20%	0.241%
28	12.469	1762	1765	1769	rVV4	61615	100391	4.29%	0.470%
29	12.516	1771	1773	1776	rVB2	47994	42078	1.80%	0.197%
30	12.592	1783	1786	1794	rBV	344939	363597	15.52%	1.701%
31	12.692	1800	1803	1807	rBV5	59331	84653	3.61%	0.396%
32	12.821	1820	1825	1830	rBV	328902	404759	17.28%	1.893%
33	12.868	1830	1833	1839	rVV3	64565	108932	4.65%	0.509%
34	12.968	1845	1850	1856	rBV	1780276	1777004	75.86%	8.311%
35	13.192	1885	1888	1890	rBV	89028	107923	4.61%	0.505%
36	14.015	2025	2028	2031	rBV2	515420	563442	24.05%	2.635%

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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

37	14.045	2031	2033	2035	rVB	178800	128799	5.50%	0.602%
38	15.057	2202	2205	2212	rVB	193383	361437	15.43%	1.690%
39	15.357	2254	2256	2263	rVB	105736	132234	5.64%	0.618%
40	15.421	2264	2267	2273	rVB	114980	158175	6.75%	0.740%
41	15.486	2274	2278	2286	rVB	390508	552583	23.59%	2.584%

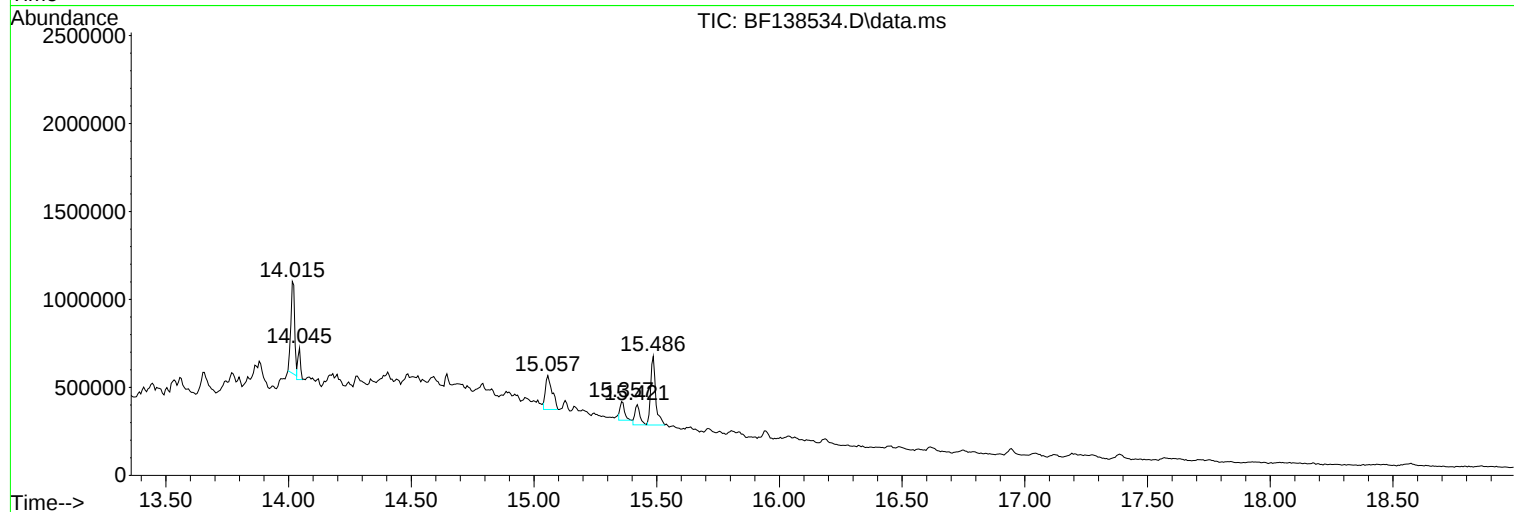
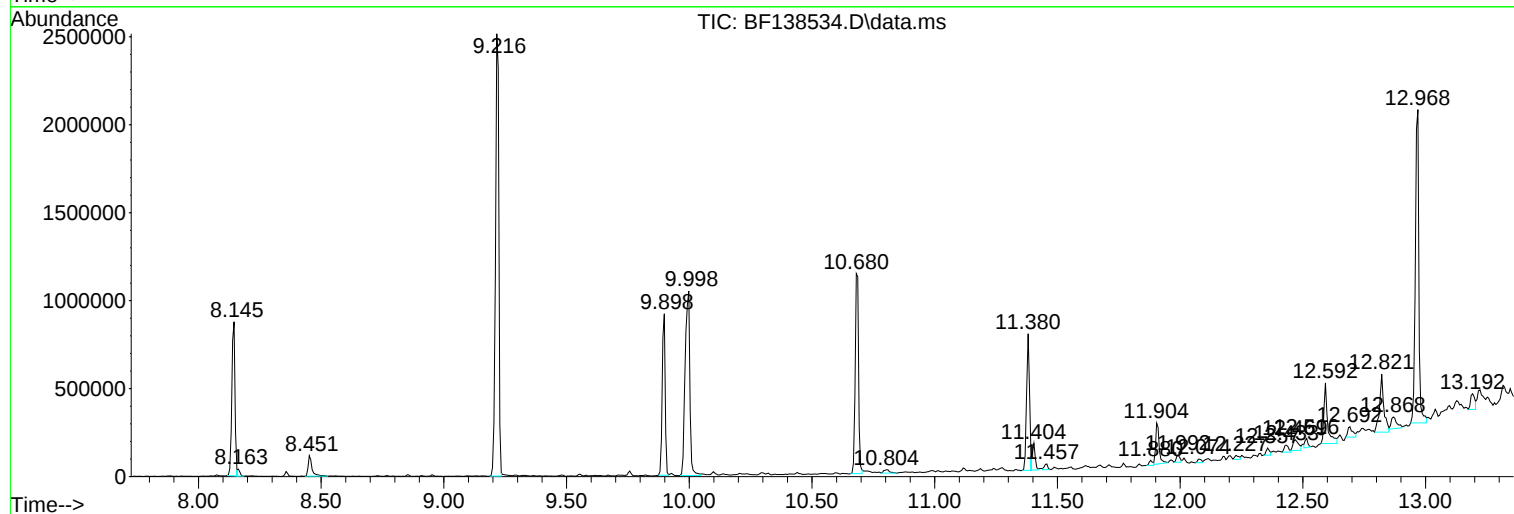
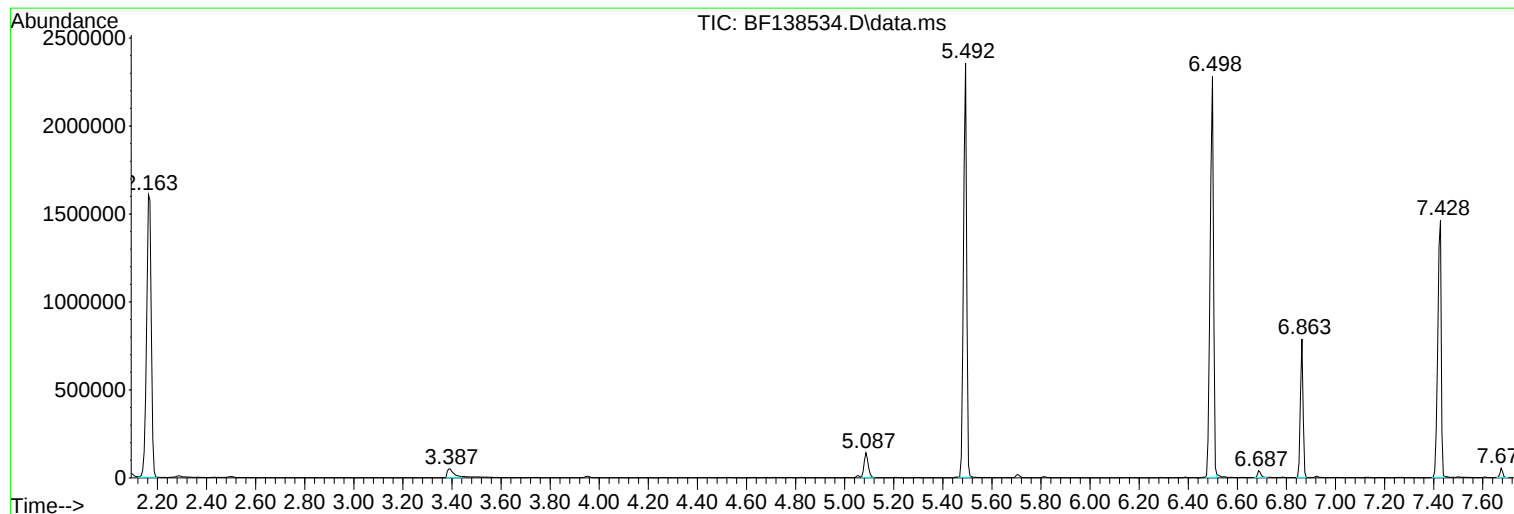
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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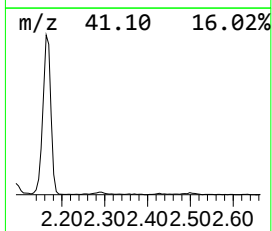
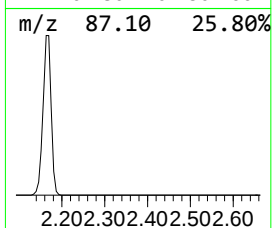
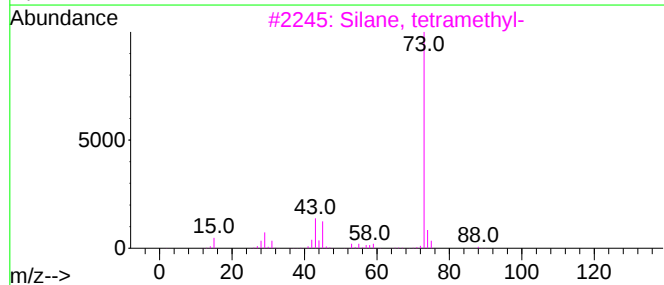
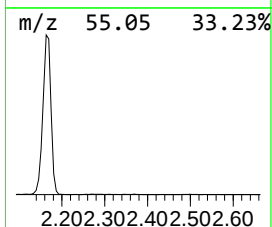
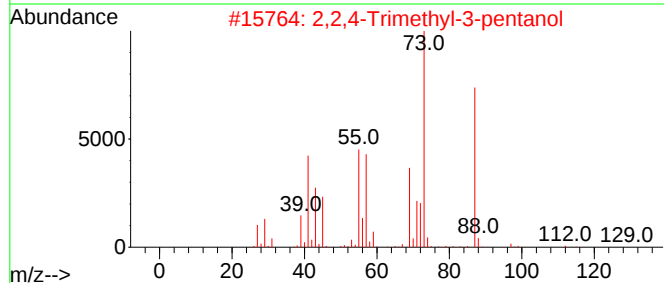
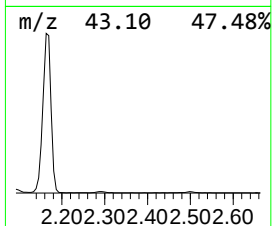
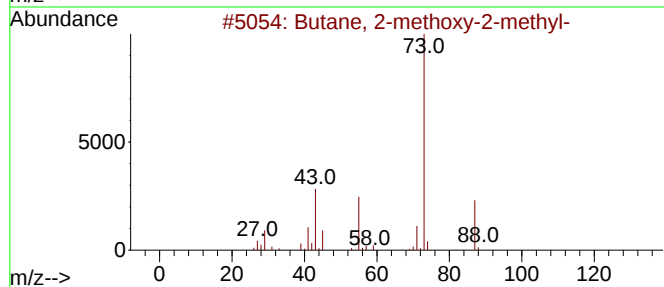
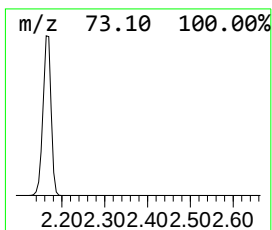
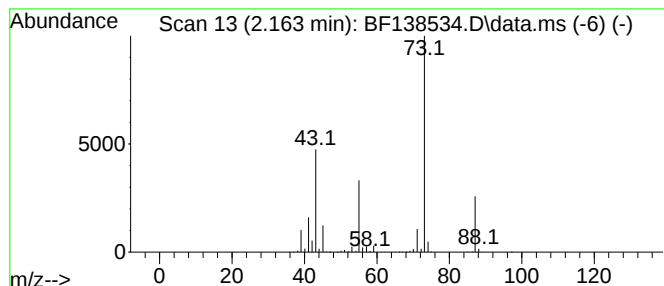
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	70.41 ng	2105450	1,4-Dichlorobenzene-d4	6.863

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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ClientSampleId :
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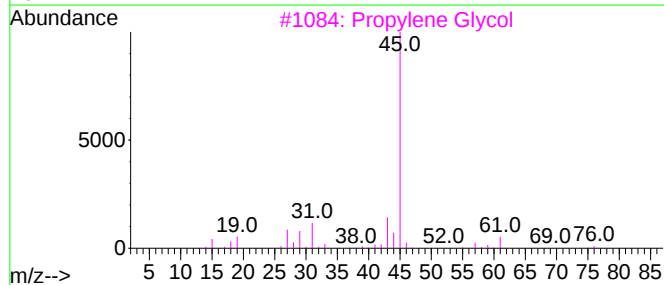
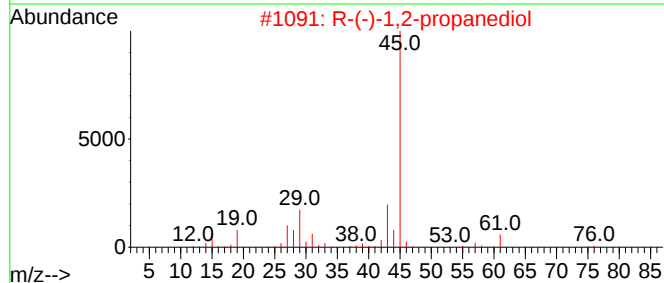
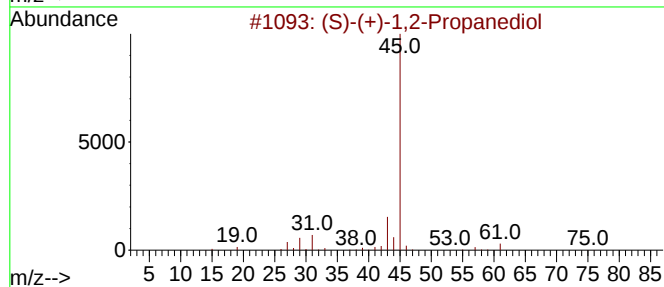
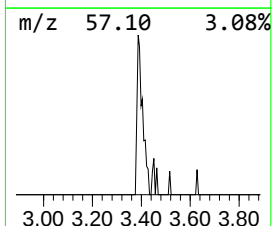
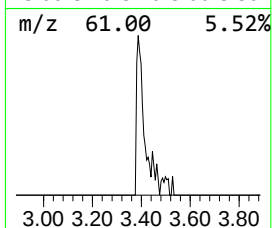
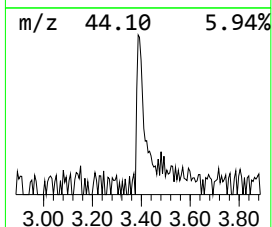
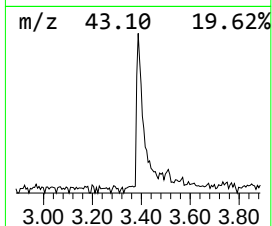
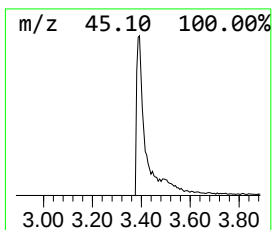
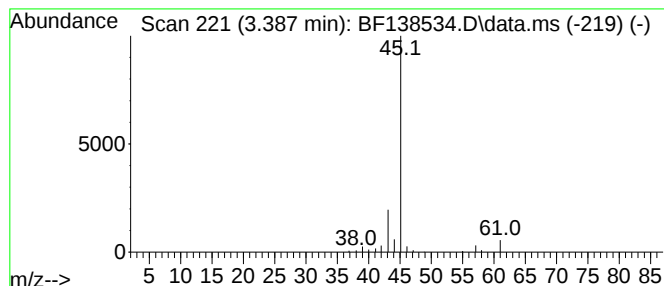
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	3.24 ng	96931	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
3	Propylene Glycol			76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol			60	C3H8O	000067-63-0	9
5	Formamide			45	CH3NO	000075-12-7	7



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ALS Vial : 20 Sample Multiplier: 1

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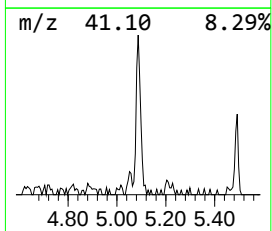
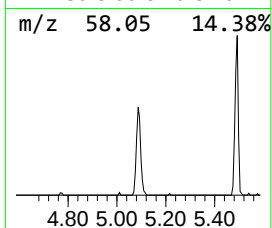
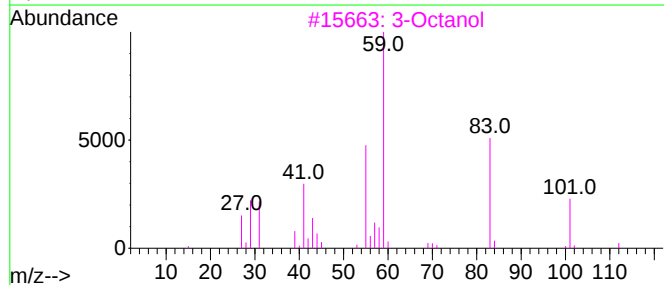
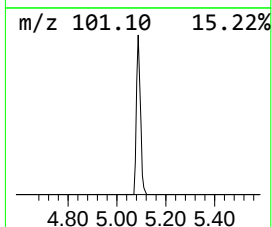
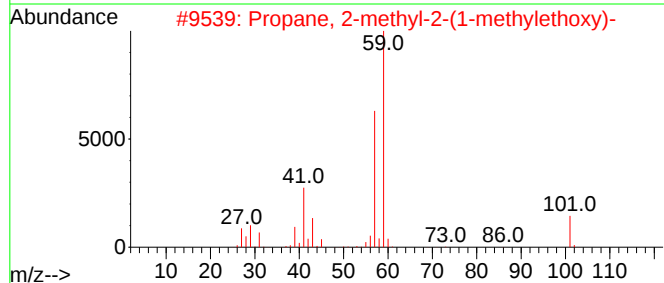
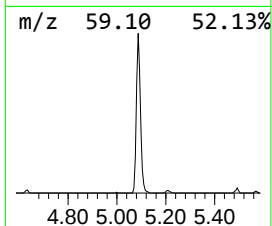
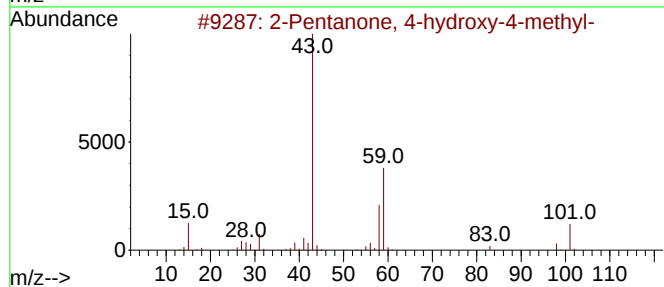
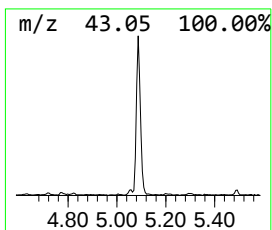
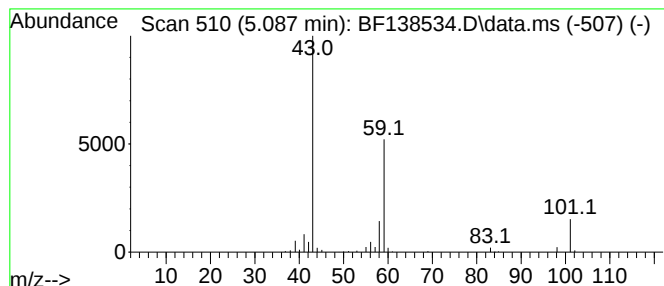
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	5.46 ng	163392	1,4-Dichlorobenzene-d4	6.863

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	3-Octanol	130	C8H18O	000589-98-0	36		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



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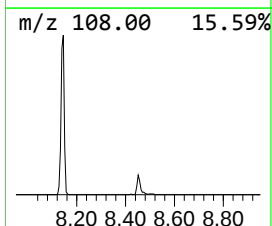
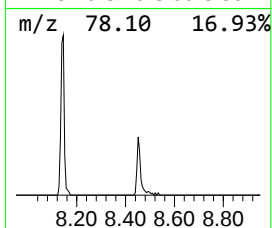
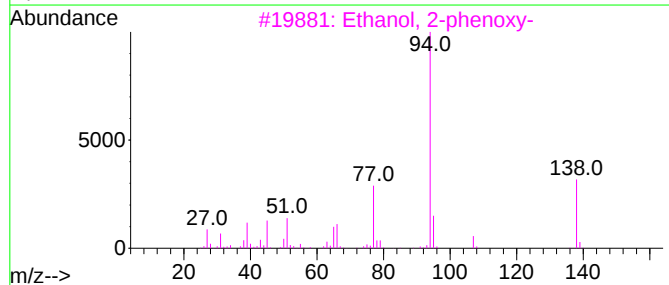
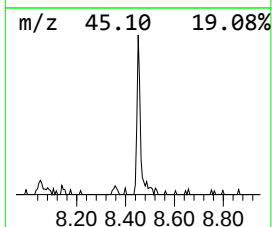
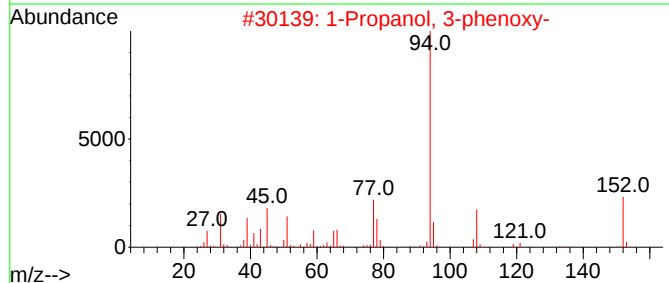
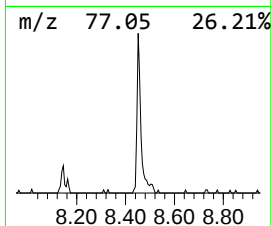
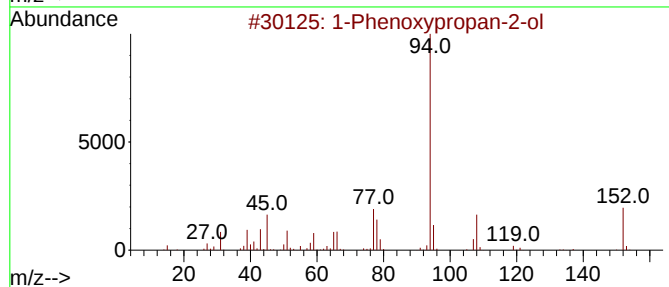
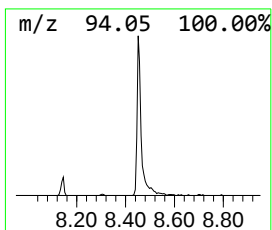
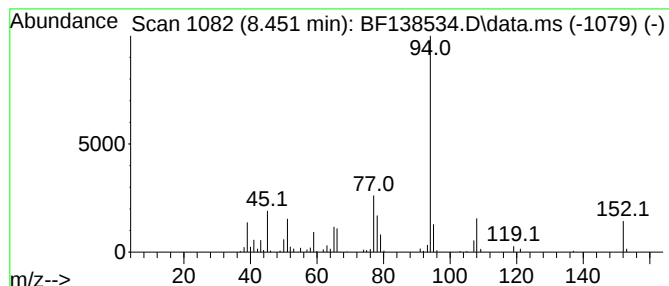
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	3.28 ng	128460	Naphthalene-d8	8.145

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	50
5		tert-Butyl phenyl carbonate	194	C11H14O3	006627-89-0	47



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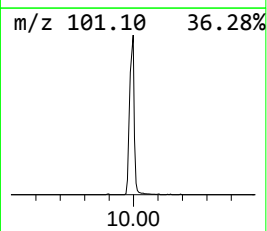
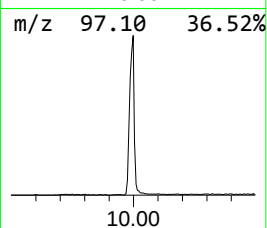
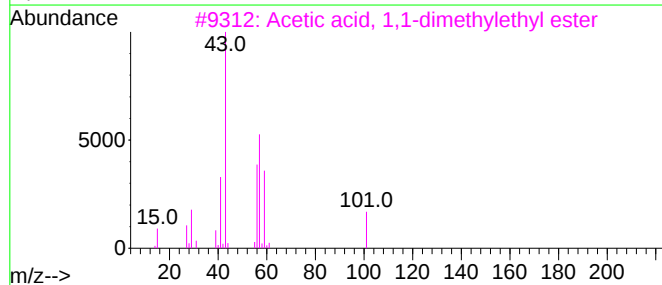
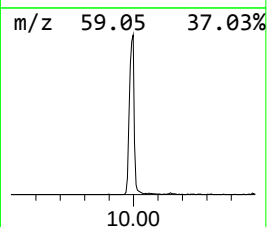
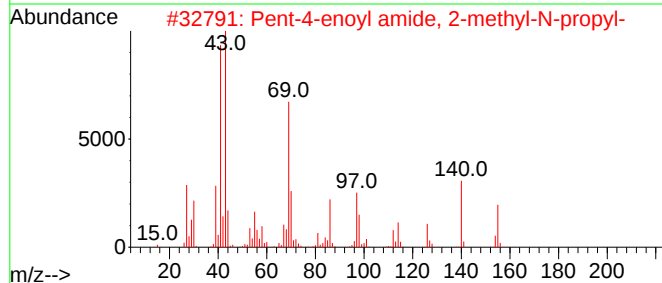
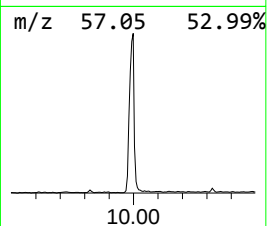
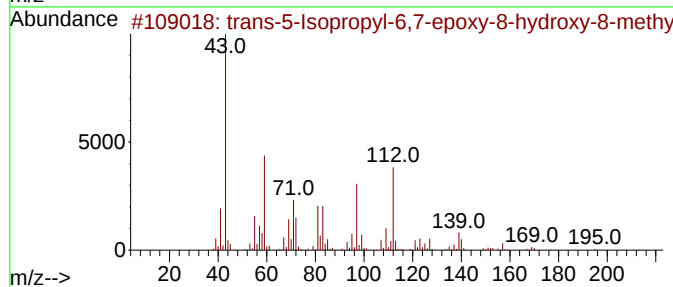
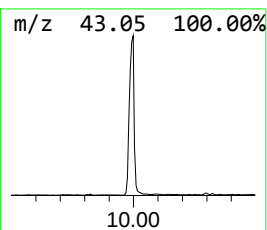
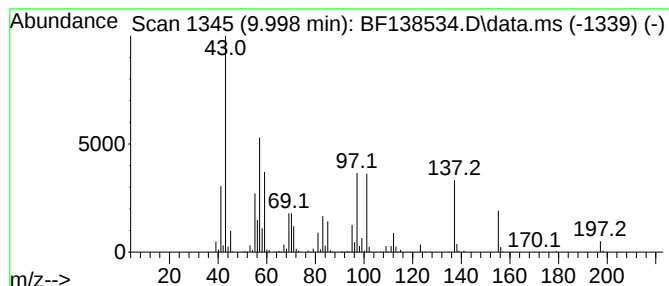
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.998 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.998	36.27 ng	1393430	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	16
2			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
4			Carbonic acid, eicosyl prop-1-en...	382	C24H46O3	1000383-10-8	10
5			2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138534.D
Acq On : 11 Jul 2024 20:52
Operator : CG\JU
Sample : P3208-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
352

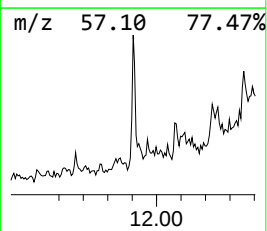
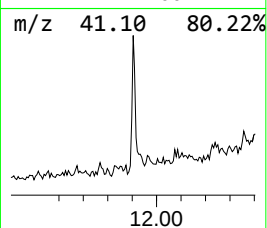
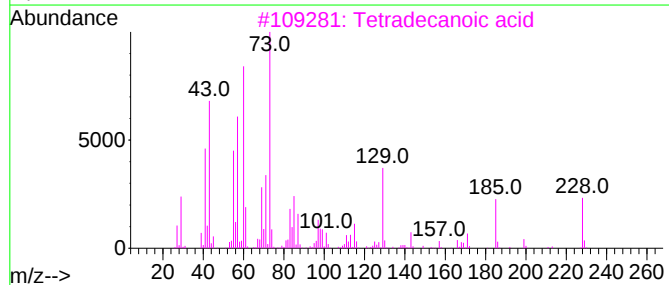
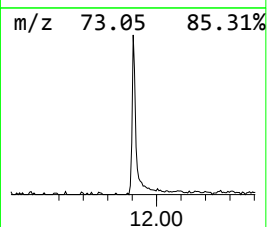
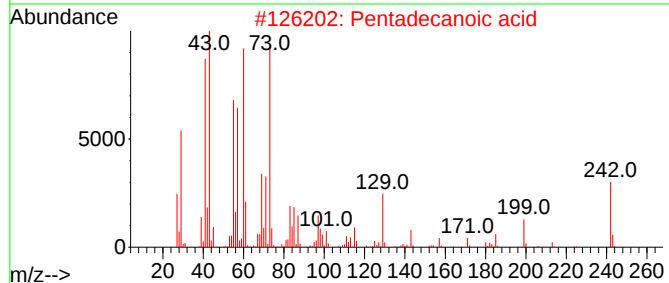
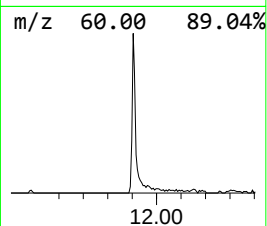
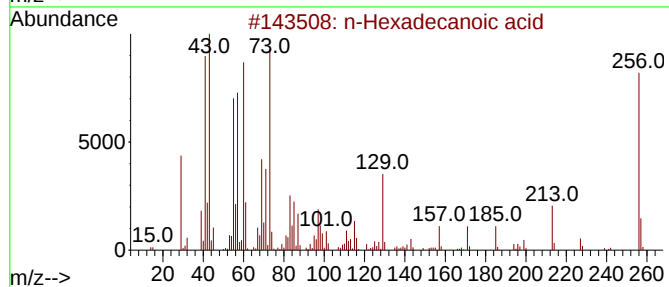
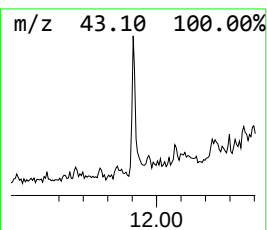
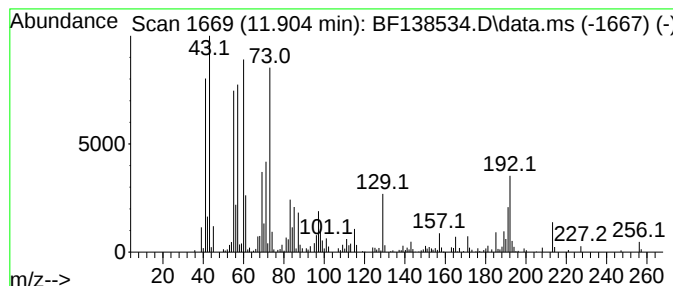
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	7.19 ng	229462	Phenanthrene-d10	11.380

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	68
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	52
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138534.D
Acq On : 11 Jul 2024 20:52
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Sample : P3208-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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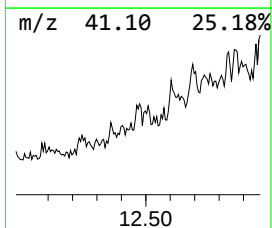
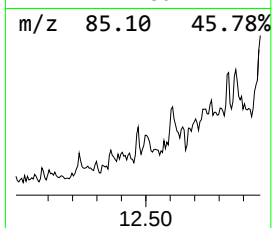
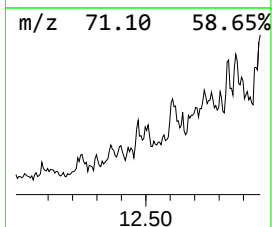
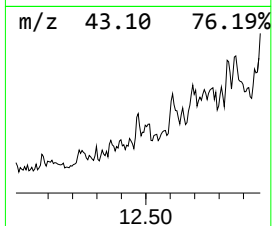
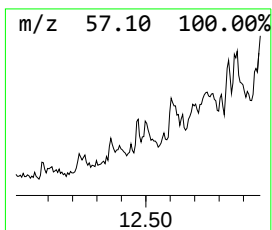
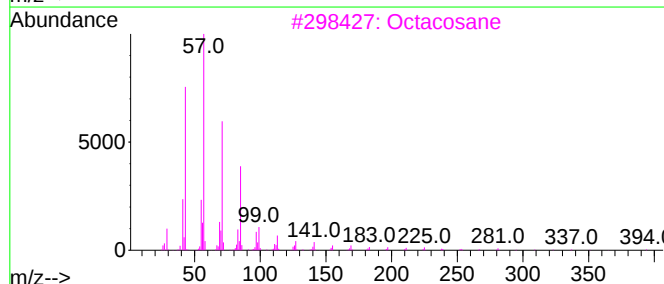
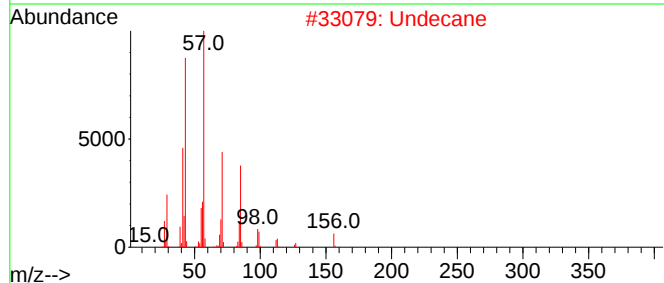
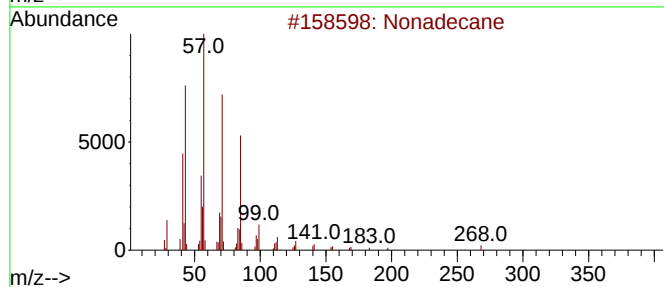
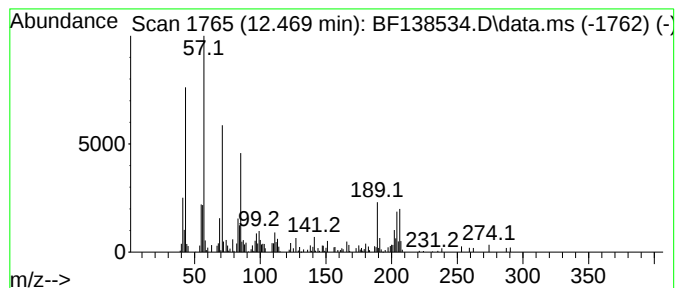
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	3.15 ng	100391	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	55
2			Undecane	156	C11H24	001120-21-4	49
3			Octacosane	394	C28H58	000630-02-4	49
4			Heptacosane	380	C27H56	000593-49-7	46
5			Hexadecane	226	C16H34	000544-76-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138534.D
Acq On : 11 Jul 2024 20:52
Operator : CG\JU
Sample : P3208-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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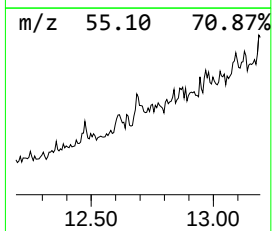
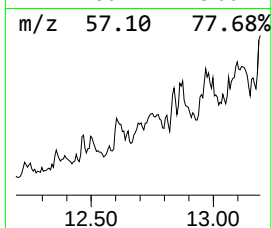
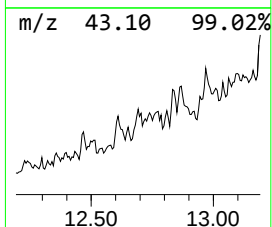
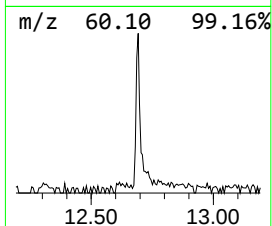
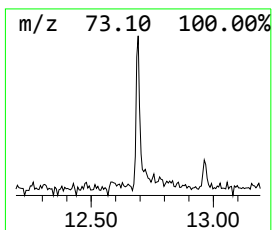
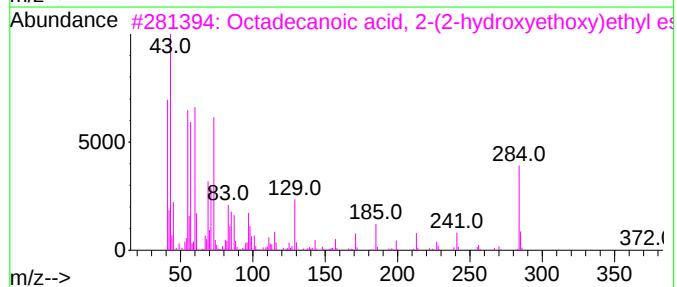
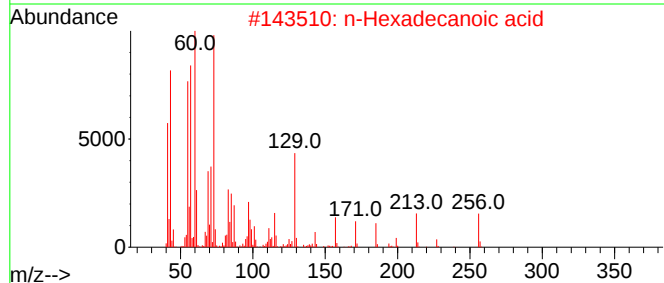
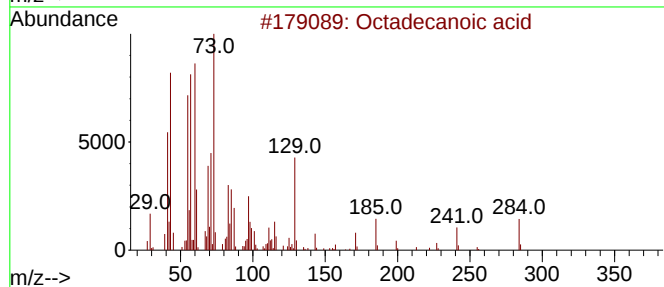
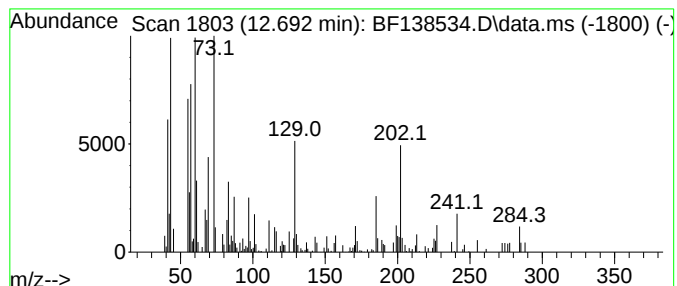
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.692	2.65 ng	84653	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	76
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	49
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138534.D
Acq On : 11 Jul 2024 20:52
Operator : CG\JU
Sample : P3208-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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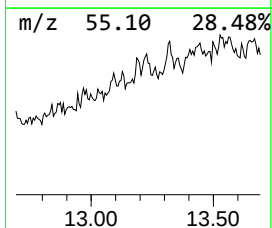
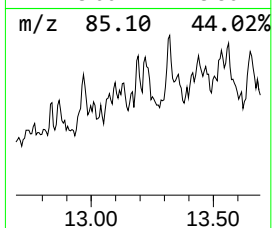
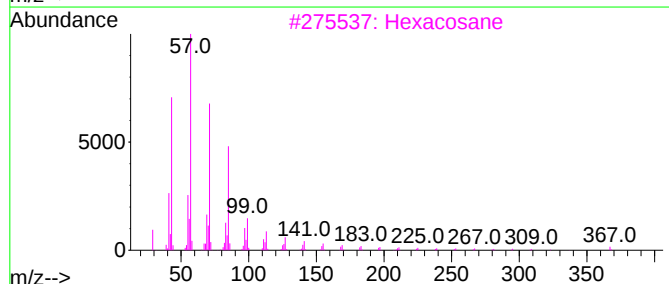
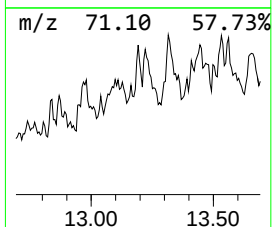
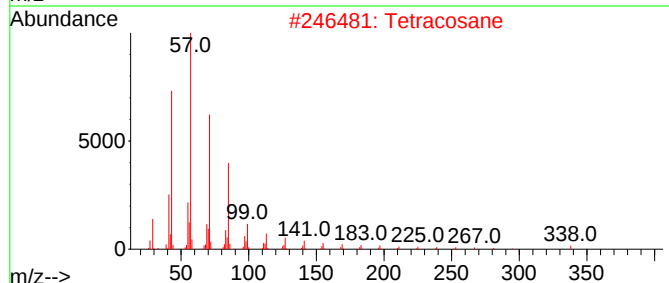
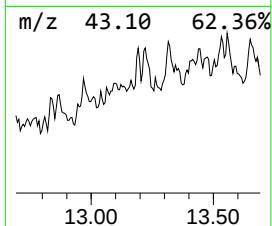
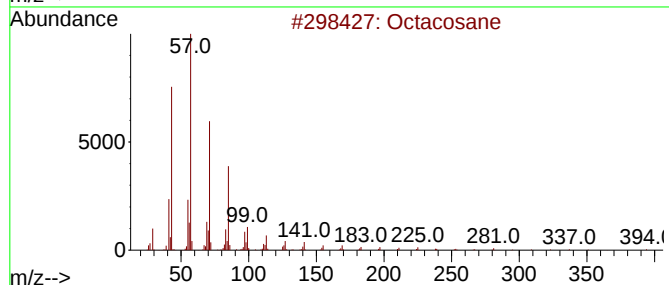
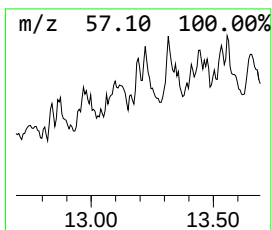
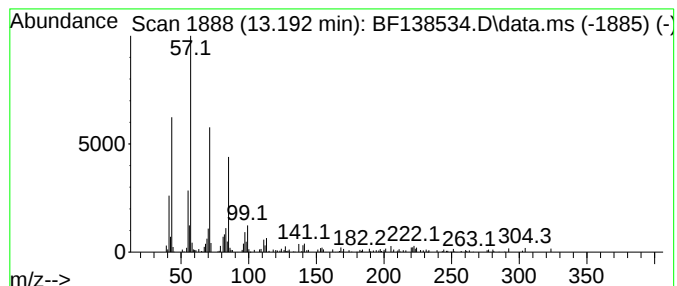
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	3.83 ng	107923	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Tetracosane	338	C24H50	000646-31-1	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Heneicosane	296	C21H44	000629-94-7	86
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138534.D
Acq On : 11 Jul 2024 20:52
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Sample : P3208-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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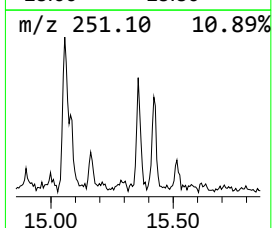
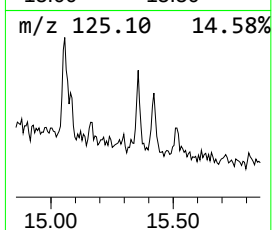
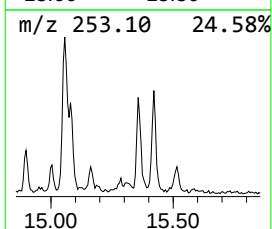
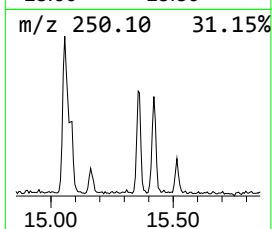
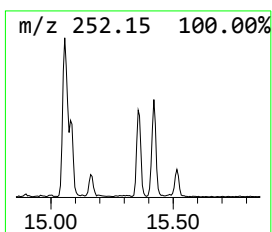
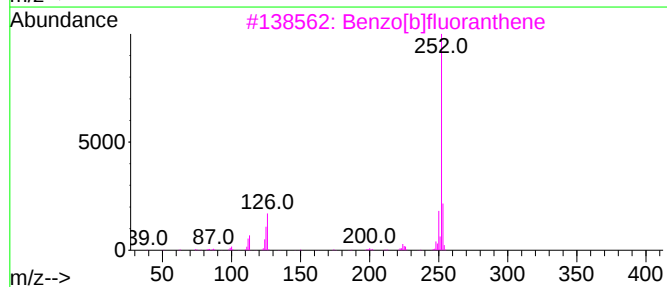
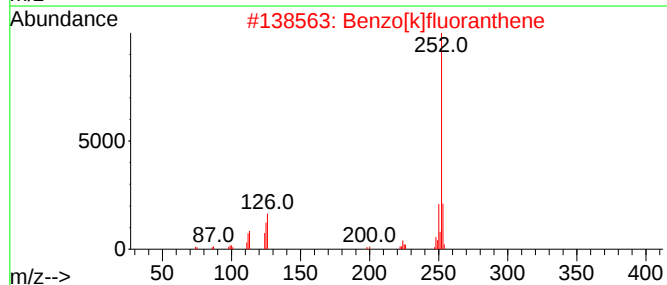
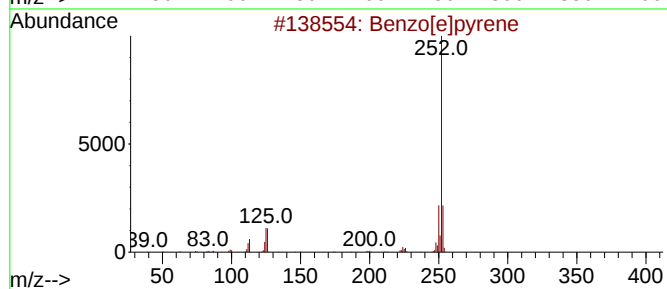
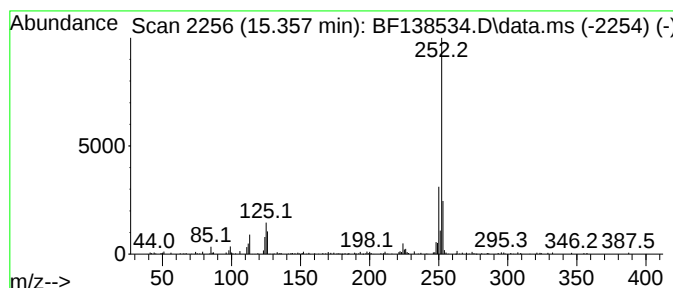
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.357	4.79 ng	132234	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Perylene	252	C20H12	000198-55-0	91
5			Benzo[a]pyrene	252	C20H12	000050-32-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138534.D
Acq On : 11 Jul 2024 20:52
Operator : CG\JU
Sample : P3208-01
Misc :
ALS Vial : 20 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\NIST20.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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(S)-(+)-1,2-Pro...	3.387	3.2	ng	96931	1	6.863	598080	20.0
2-Pentanone, 4-...	5.087	5.5	ng	163392	1	6.863	598080	20.0
1-Phenoxypropan...	8.451	3.3	ng	128460	2	8.145	783824	20.0
unknown9.998	9.998	36.3	ng	1393430	3	9.898	768318	20.0
n-Hexadecanoic ...	11.904	7.2	ng	229462	4	11.380	638255	20.0
Nonadecane	12.469	3.1	ng	100391	4	11.380	638255	20.0
Octadecanoic acid	12.692	2.6	ng	84653	4	11.380	638255	20.0
Octacosane	13.192	3.8	ng	107923	5	14.021	563442	20.0
Benzo[e]pyrene	15.357	4.8	ng	132234	6	15.486	552583	20.0