

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081224\
 Data File : BF138935.D
 Acq On : 12 Aug 2024 15:46
 Operator : RC/JU
 Sample : P3512-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 931-K1-SD-0-0.5-080724-FD

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-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138935.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.416	220	225	243	rBV	3109	14048	1.63%	0.244%
2	5.057	500	504	518	rVB	32287	50908	5.91%	0.886%
3	5.469	569	574	596	rBV	564910	786967	91.31%	13.695%
4	6.481	741	746	771	rBV	601630	823119	95.51%	14.324%
5	6.839	802	807	813	rVB	185046	227933	26.45%	3.966%
6	7.404	898	903	921	rBV	407289	521178	60.47%	9.070%
7	7.663	944	947	955	rBV	7489	13129	1.52%	0.228%
8	8.122	1020	1025	1041	rBV	228895	300740	34.89%	5.233%
9	8.439	1075	1079	1097	rBV	25057	41469	4.81%	0.722%
10	9.192	1202	1207	1217	rBV	691947	861850	100.00%	14.998%
11	9.869	1317	1322	1334	rBV	256320	328685	38.14%	5.720%
12	9.963	1334	1338	1346	rVB	13792	20114	2.33%	0.350%
13	10.663	1452	1457	1471	rBV	337047	449460	52.15%	7.821%
14	11.357	1570	1575	1585	rBV	234760	299792	34.78%	5.217%
15	12.939	1838	1844	1853	rBV	422383	538206	62.45%	9.366%
16	13.839	1990	1997	2013	rBV5	8781	29476	3.42%	0.513%
17	13.998	2019	2024	2032	rBV	110624	146894	17.04%	2.556%
18	15.080	2203	2208	2213	rBV	29878	40320	4.68%	0.702%
19	15.462	2267	2273	2286	rBV	107318	176676	20.50%	3.075%
20	15.657	2300	2306	2311	rBV2	12587	21140	2.45%	0.368%
21	15.880	2338	2344	2351	rVB	21398	35082	4.07%	0.610%
22	16.668	2472	2478	2488	rVB4	8721	19290	2.24%	0.336%

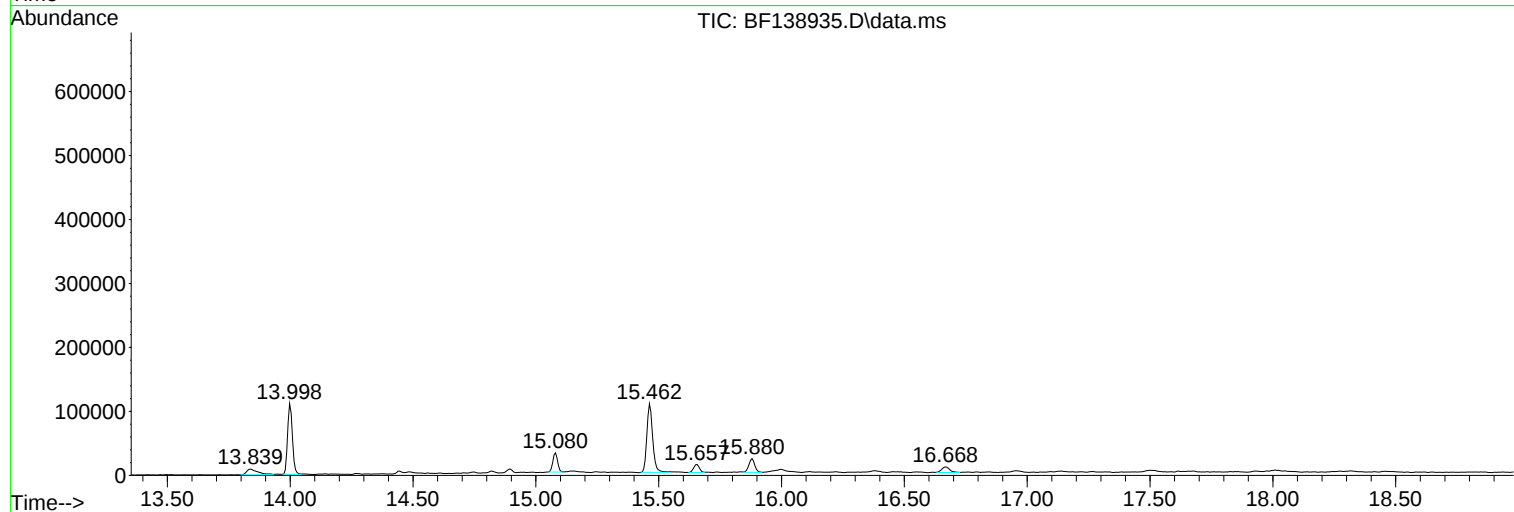
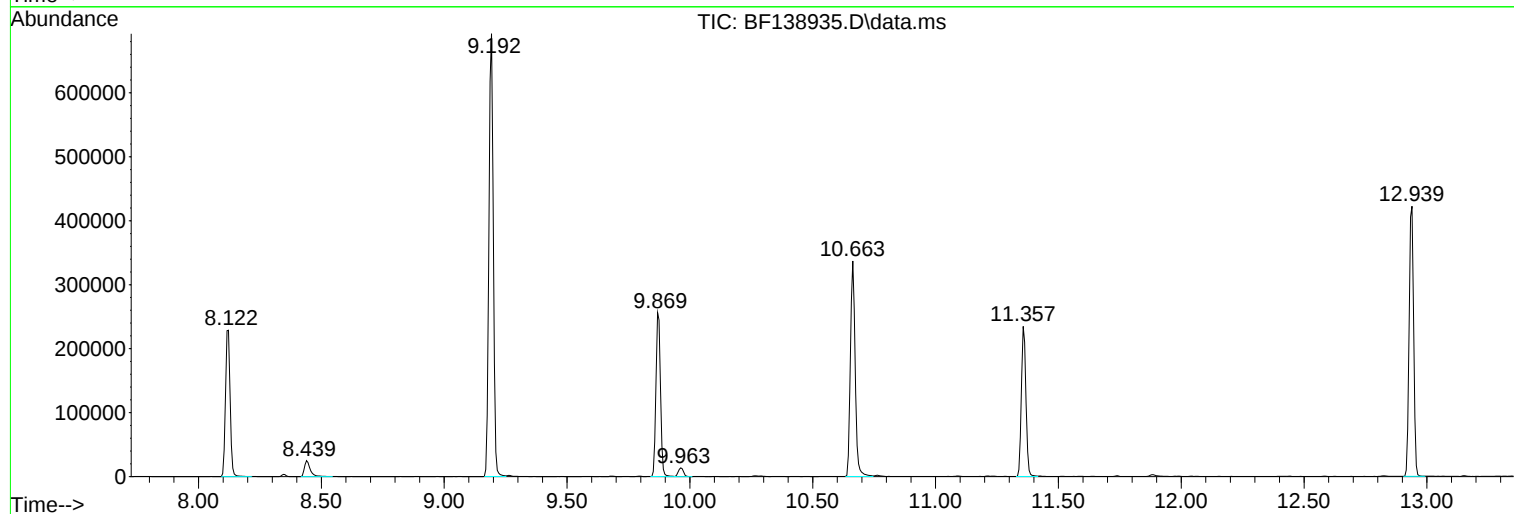
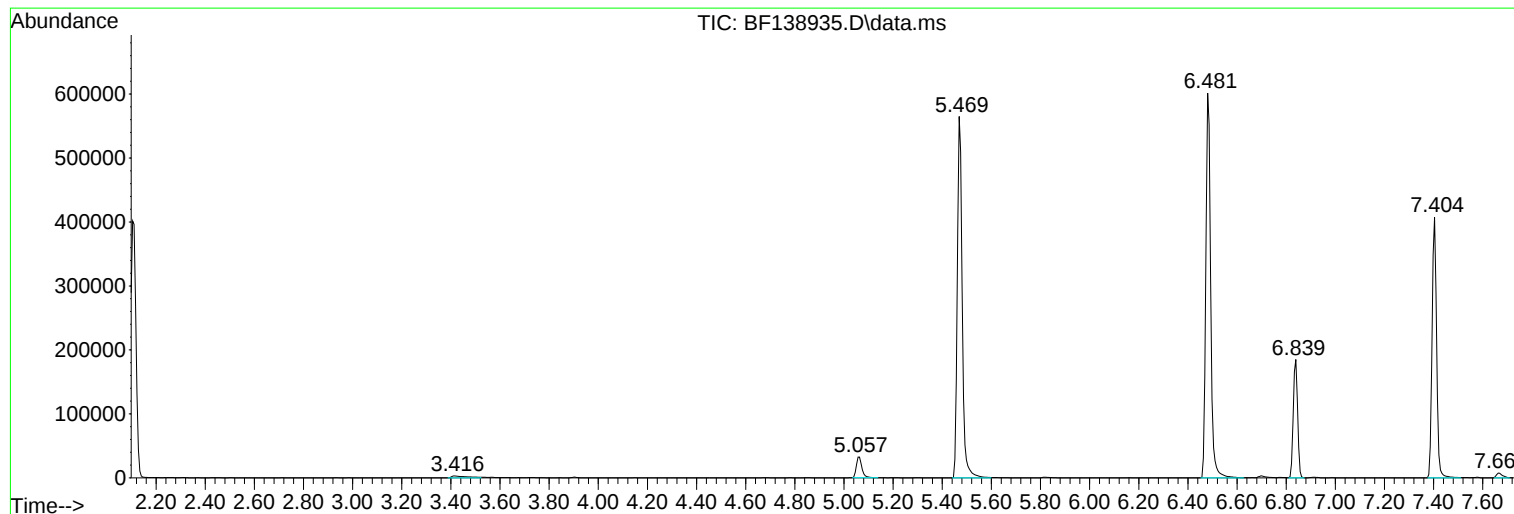
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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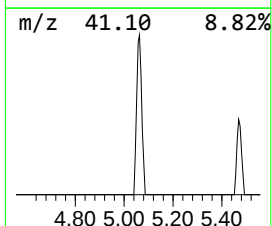
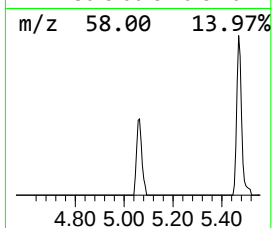
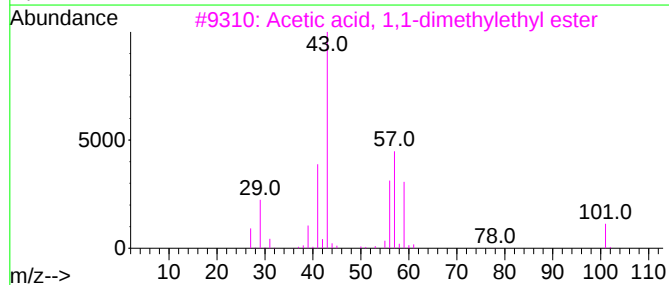
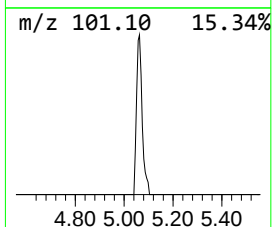
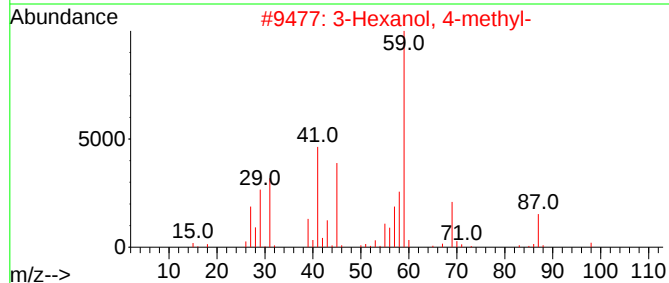
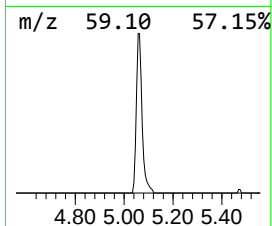
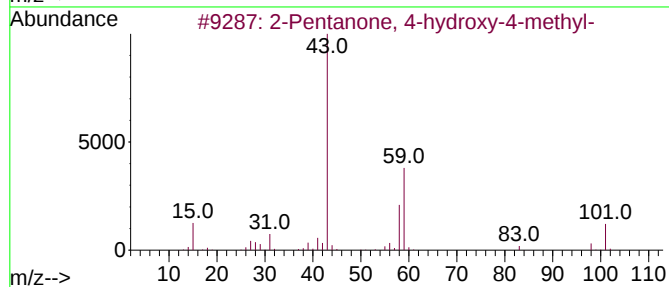
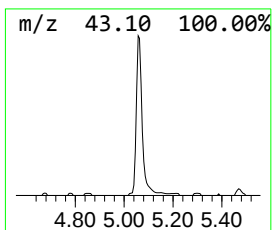
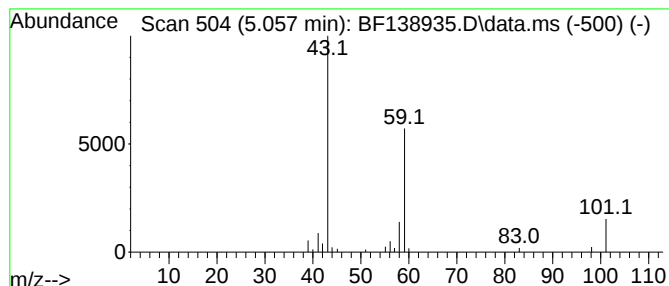
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	4.47 ng	50908	1,4-Dichlorobenzene-d4	6.839

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9	



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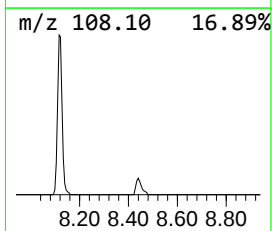
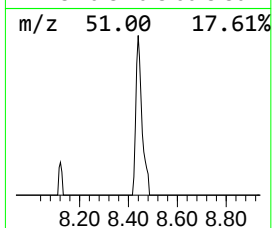
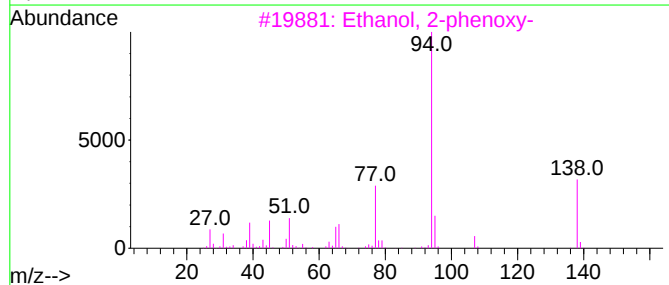
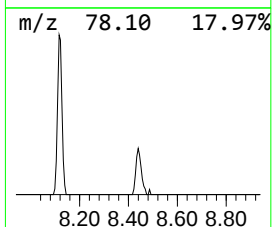
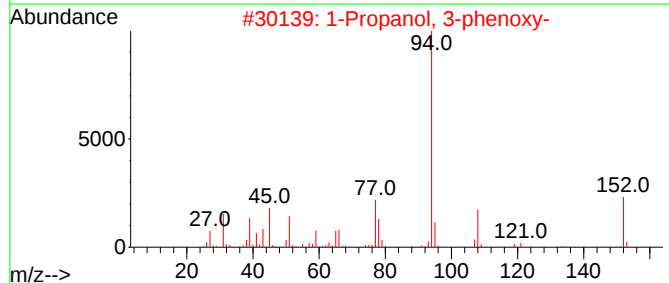
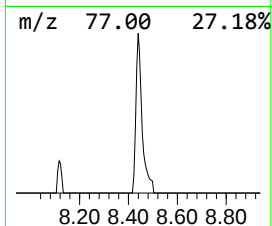
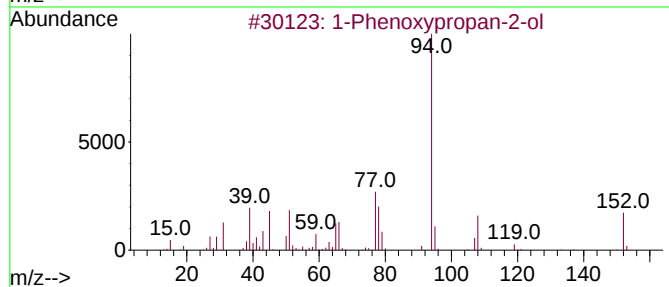
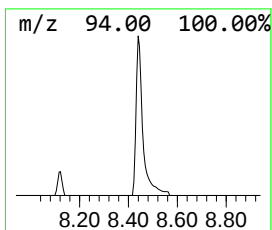
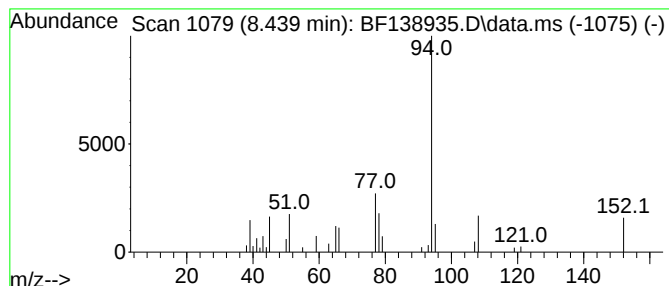
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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.439	2.76 ng	41469	Naphthalene-d8	8.122

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		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5		Benzene, propoxy-	136	C9H12O	000622-85-5	53



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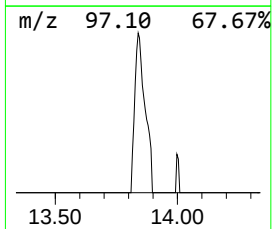
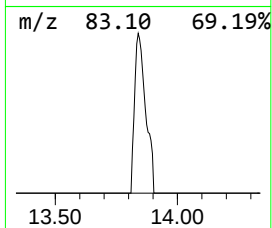
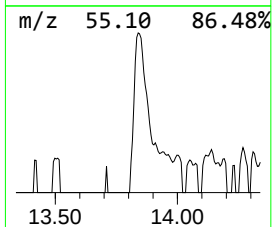
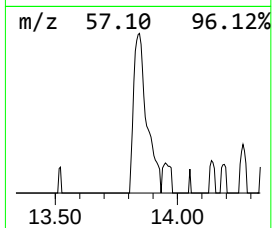
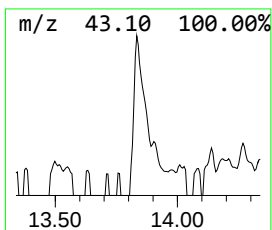
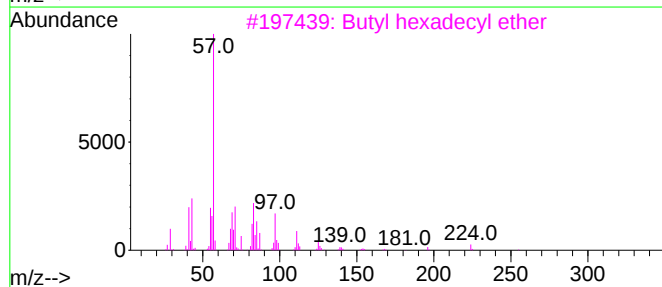
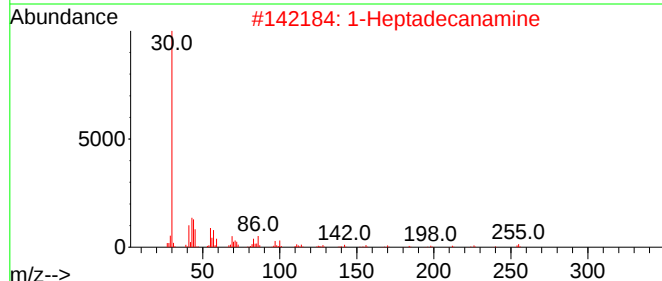
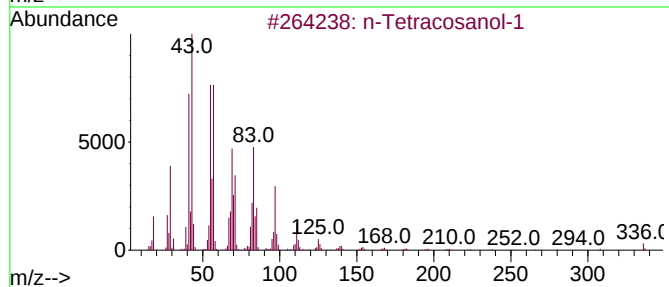
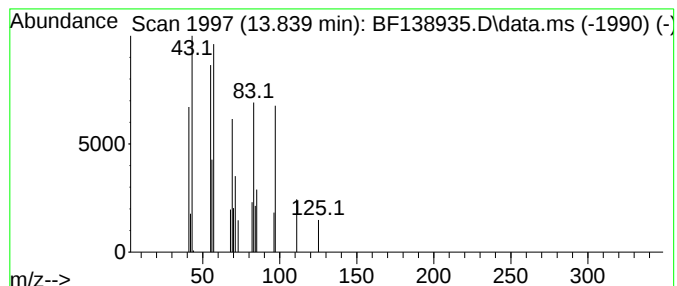
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	4.01 ng	29476	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	72
2			1-Heptadecanamine	255	C17H37N	004200-95-7	64
3			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	59
4			Butyl docosyl ether	382	C26H54O	1000406-40-8	59
5			n-Tridecan-1-ol	200	C13H28O	000112-70-9	59



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Misc :
ALS Vial : 13 Sample Multiplier: 1

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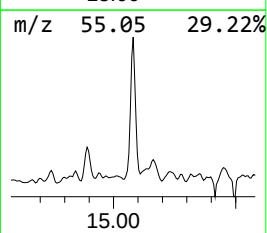
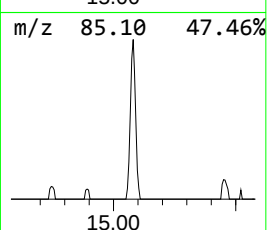
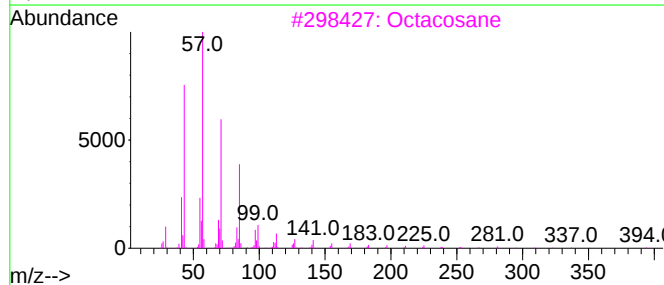
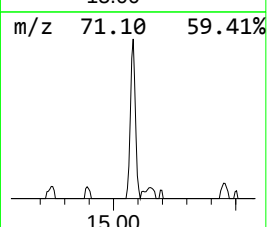
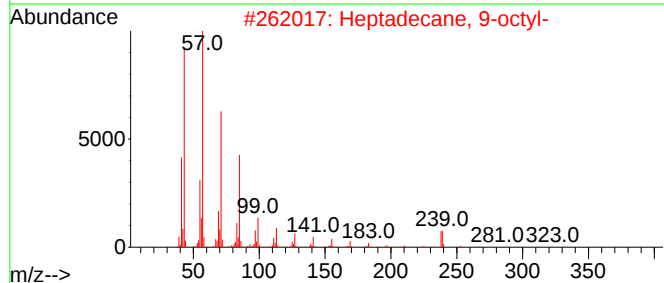
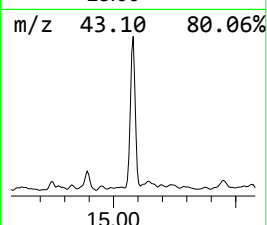
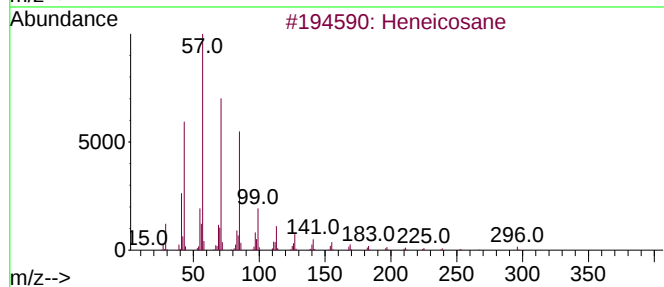
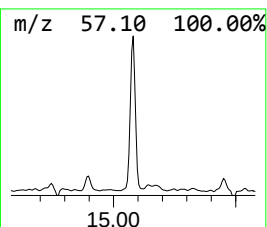
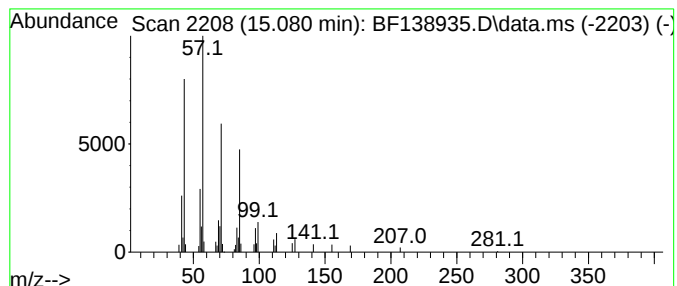
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Peak Number 4 Heneicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	4.56 ng	40320	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Eicosane, 9-octyl-	394	C28H58	013475-77-9	91
5			Hexacosane	366	C26H54	000630-01-3	90



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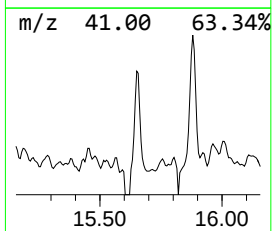
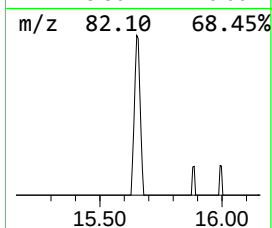
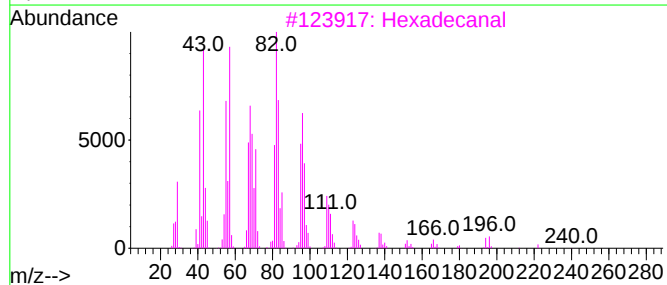
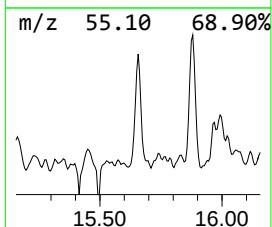
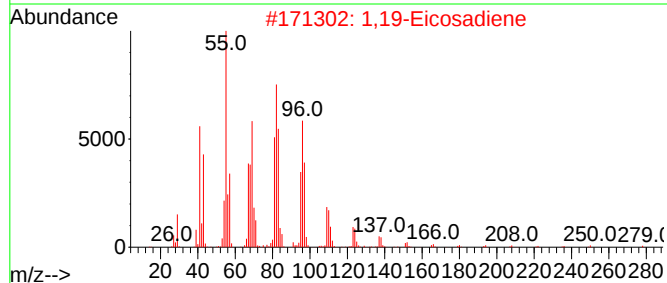
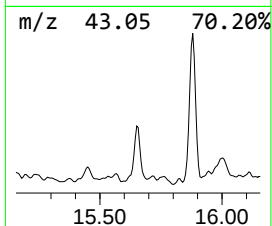
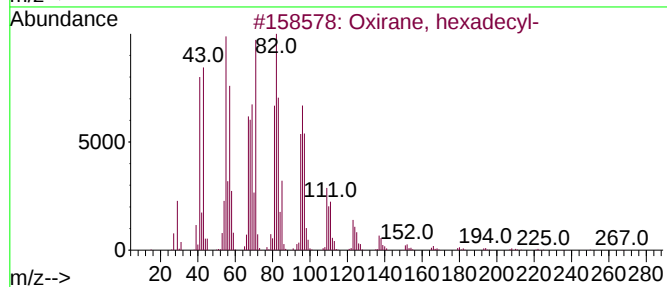
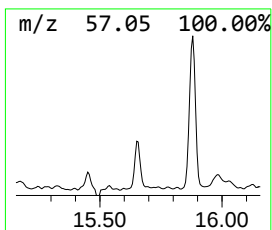
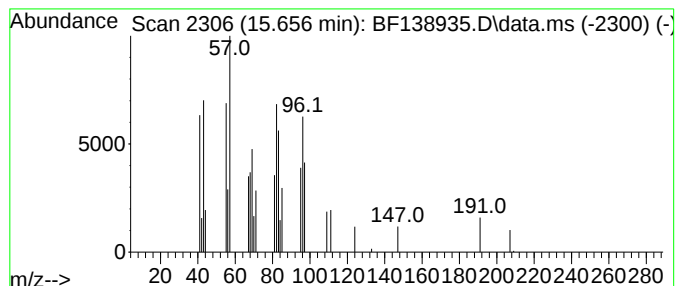
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.656	2.39 ng	21140	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	64
2			1,19-Eicosadiene	278	C20H38	014811-95-1	64
3			Hexadecanal	240	C16H32O	000629-80-1	52
4			Pentadecanal-	226	C15H30O	002765-11-9	50
5			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	50



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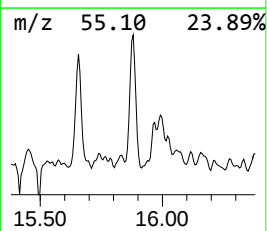
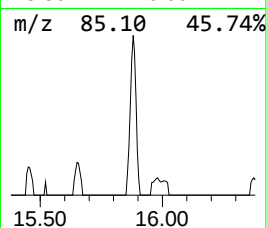
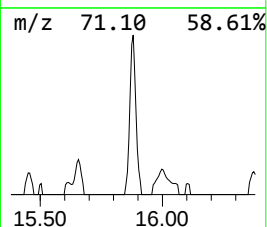
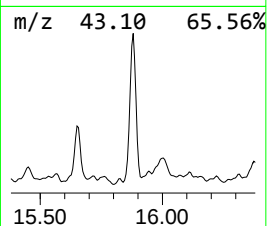
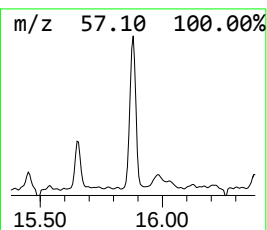
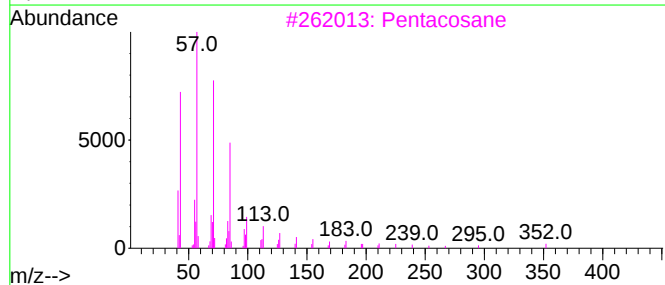
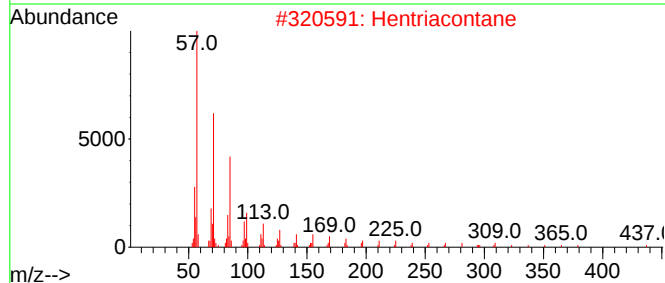
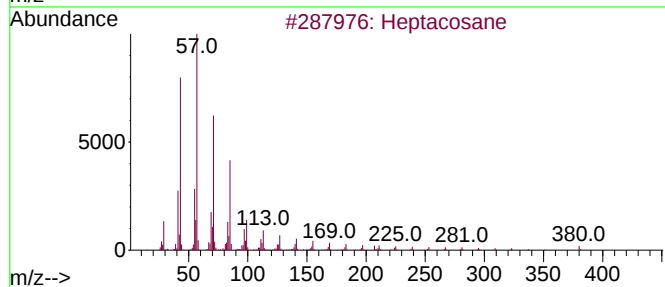
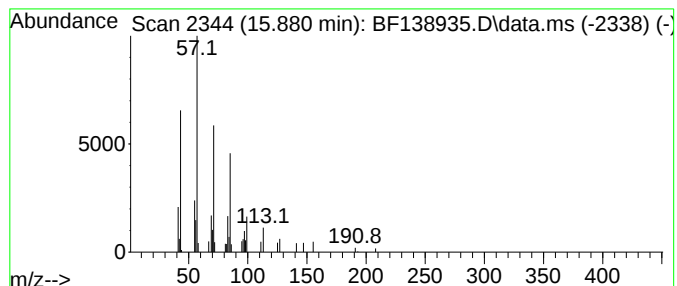
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.880	3.97 ng	35082	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			Tetratetracontane	619	C44H90	007098-22-8	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081224\
Data File : BF138935.D
Acq On : 12 Aug 2024 15:46
Operator : RC/JU
Sample : P3512-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
931-K1-SD-0-0.5-080724-FD

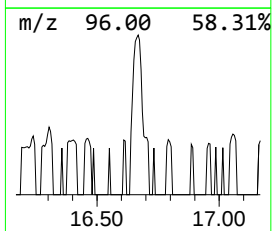
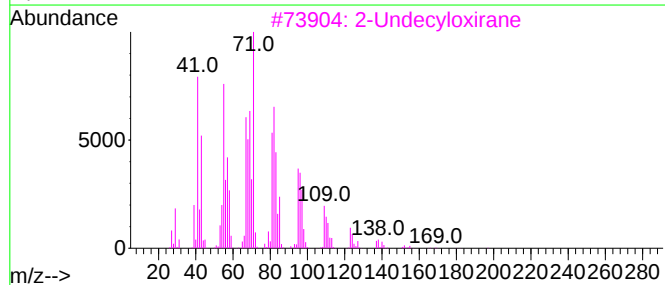
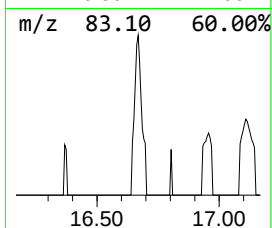
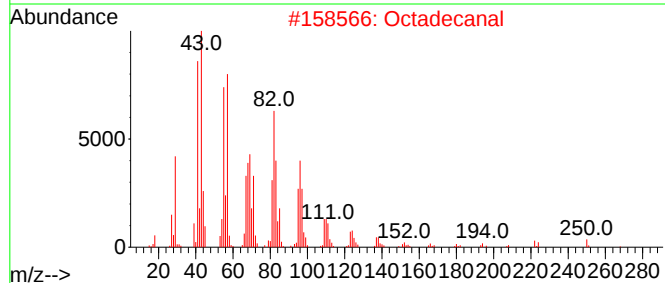
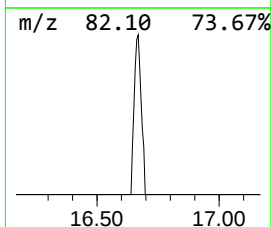
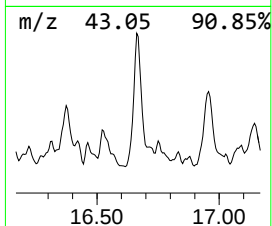
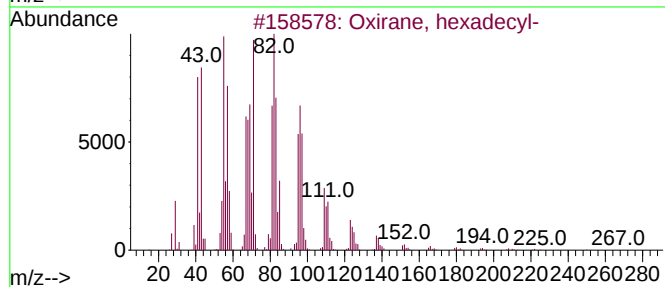
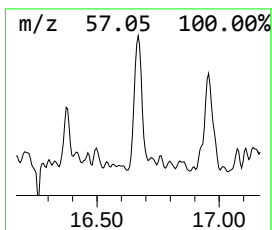
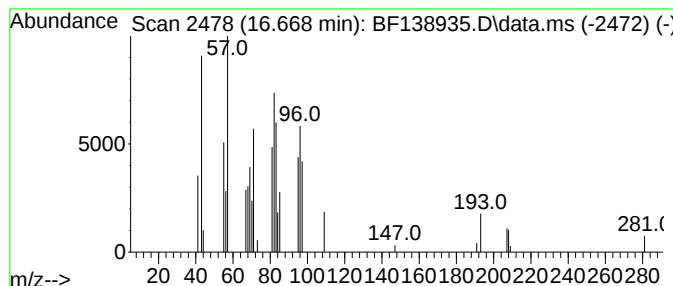
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.668	2.18 ng	19290	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	86	
2	Octadecanal		268	C18H36O	000638-66-4	86	
3	2-Undecyloxirane		198	C13H26O	001713-31-1	72	
4	1,19-Eicosadiene		278	C20H38	014811-95-1	59	
5	1-Cyclohexylnonene		208	C15H28	114614-84-5	49	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081224\
Data File : BF138935.D
Acq On : 12 Aug 2024 15:46
Operator : RC/JU
Sample : P3512-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
931-K1-SD-0-0.5-080724-FD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.057	4.5	ng	50908	1	6.839	227933	20.0
1-Phenoxypropan...	8.439	2.8	ng	41469	2	8.122	300740	20.0
n-Tetracosanol-1	13.839	4.0	ng	29476	5	13.998	146894	20.0
Heneicosane	15.080	4.6	ng	40320	6	15.462	176676	20.0
Oxirane, hexade...	15.656	2.4	ng	21140	6	15.462	176676	20.0
Heptacosane	15.880	4.0	ng	35082	6	15.462	176676	20.0
Octadecanal	16.668	2.2	ng	19290	6	15.462	176676	20.0