

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
 Data File : BF136386.D
 Acq On : 04 Dec 2023 17:27
 Operator : CG\JU
 Sample : 05434-15
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-8

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-BF112723.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136386.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	14	rVB	286052	371423	9.32%	1.568%
2	5.057	498	505	511	rVB	62485	81768	2.05%	0.345%
3	5.445	566	571	574	rBV	3298934	3132762	78.62%	13.226%
4	6.440	735	740	743	rBV	2638722	3103550	77.88%	13.103%
5	6.804	798	802	805	rBV	811778	710483	17.83%	3.000%
6	7.363	891	897	900	rBV	2136733	2011075	50.47%	8.491%
7	8.081	1014	1019	1022	rBV	995789	928354	23.30%	3.919%
8	9.157	1197	1202	1205	rBV	4540286	3984898	100.00%	16.824%
9	9.557	1268	1270	1273	rVB	78348	63130	1.58%	0.267%
10	9.833	1313	1317	1321	rVB	1173633	940906	23.61%	3.972%
11	10.627	1448	1452	1455	rBV	2187023	1836132	46.08%	7.752%
12	10.757	1470	1474	1477	rBV	82107	80710	2.03%	0.341%
13	11.327	1567	1571	1574	rBV	935679	794866	19.95%	3.356%
14	11.863	1658	1662	1671	rBV2	211170	223607	5.61%	0.944%
15	12.592	1783	1786	1790	rVB	95830	83187	2.09%	0.351%
16	12.651	1793	1796	1801	rBV4	65232	75568	1.90%	0.319%
17	12.751	1809	1813	1815	rBV	252715	233248	5.85%	0.985%
18	12.927	1838	1843	1846	rBV	3527311	3202554	80.37%	13.521%
19	13.163	1880	1883	1887	rVB	46923	44985	1.13%	0.190%
20	13.463	1930	1934	1937	rBV	185898	172043	4.32%	0.726%
21	13.839	1995	1998	1999	rBV	59722	62808	1.58%	0.265%
22	13.857	1999	2001	2008	rVB2	74091	125238	3.14%	0.529%
23	13.980	2018	2022	2025	rBV	792953	712669	17.88%	3.009%
24	14.157	2049	2052	2056	rVB	67352	53262	1.34%	0.225%
25	14.463	2101	2104	2107	rBV	83449	80399	2.02%	0.339%
26	14.774	2155	2157	2165	rVB2	61484	63778	1.60%	0.269%
27	15.462	2270	2274	2280	rBV	444948	512301	12.86%	2.163%

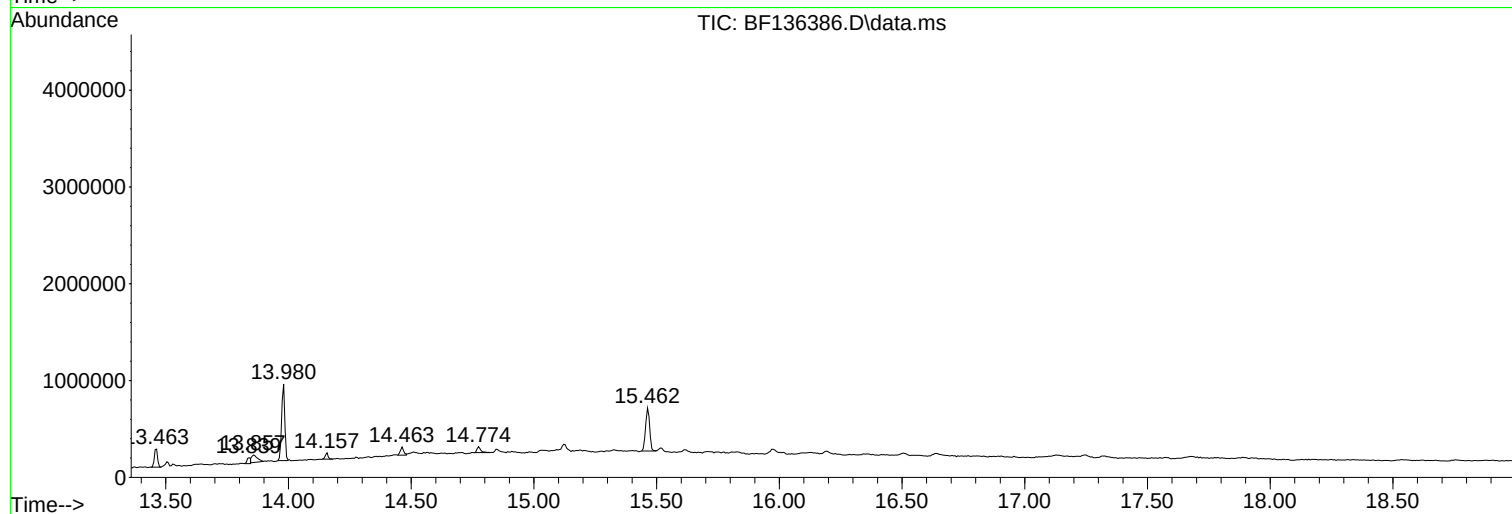
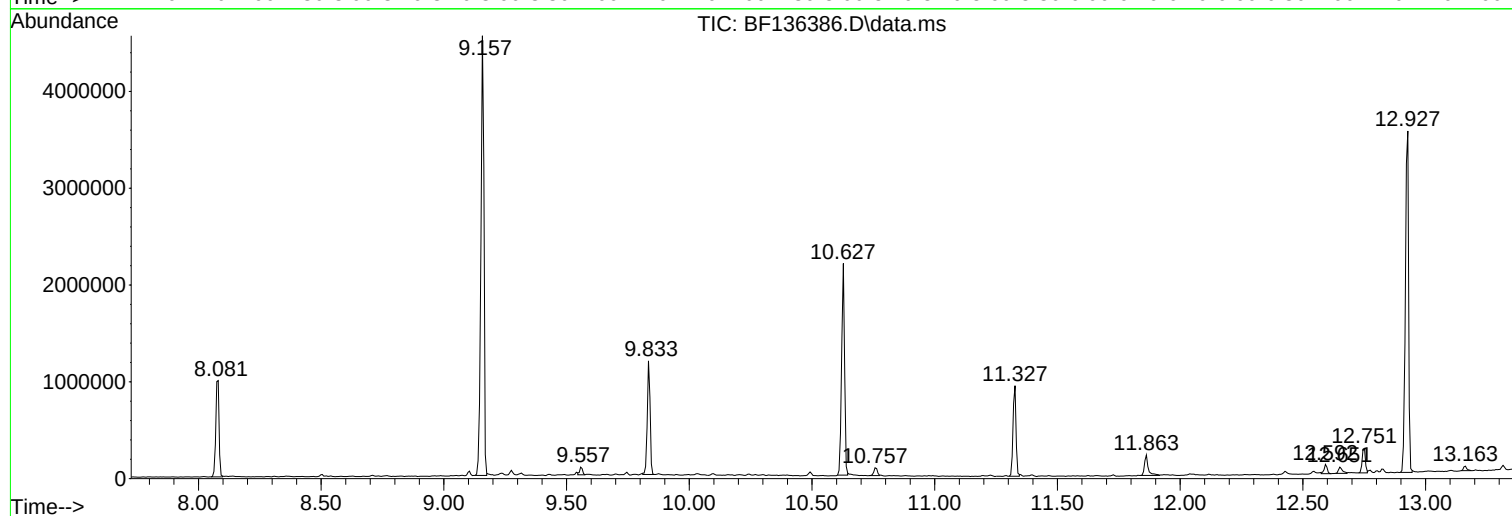
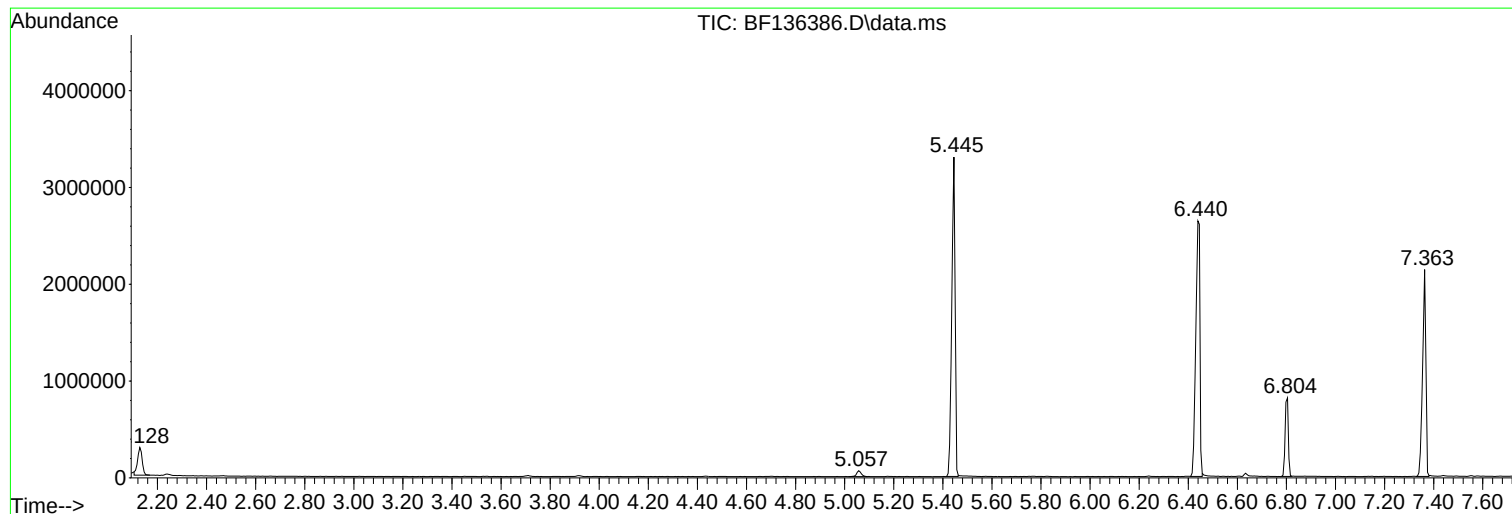
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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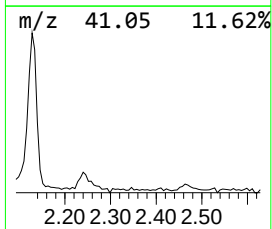
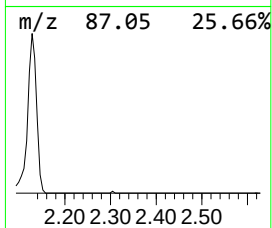
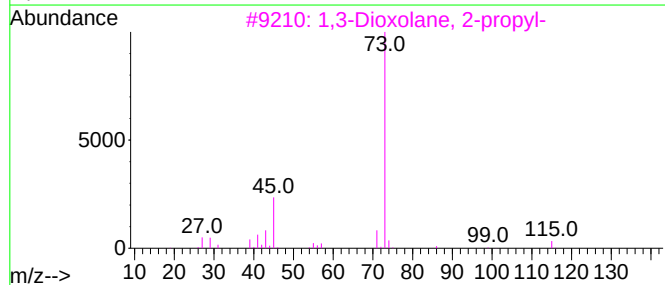
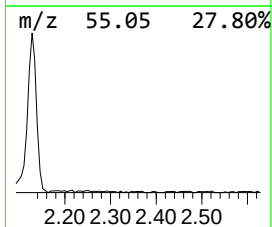
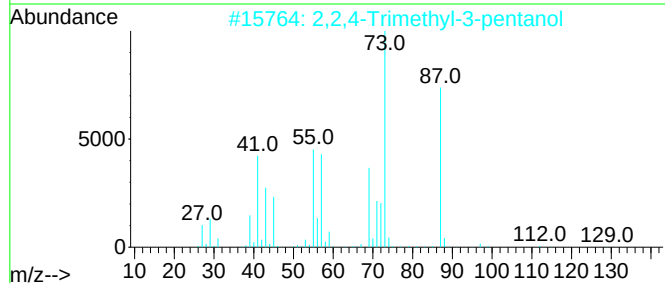
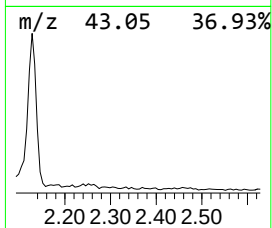
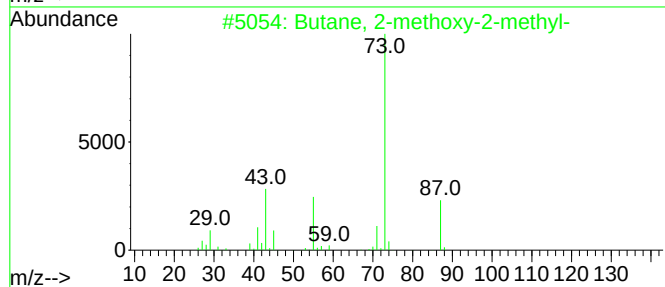
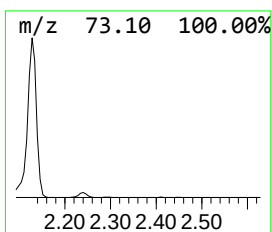
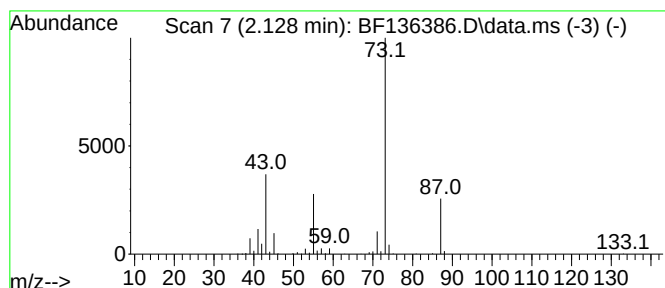
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.128	10.46 ng	371423	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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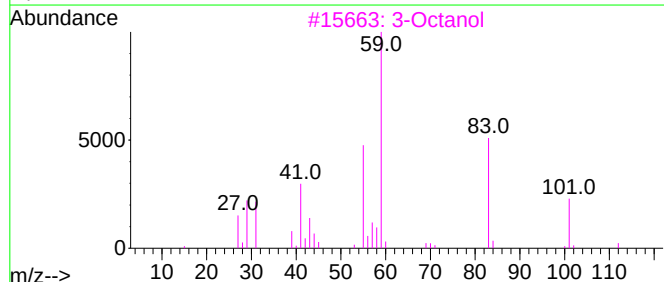
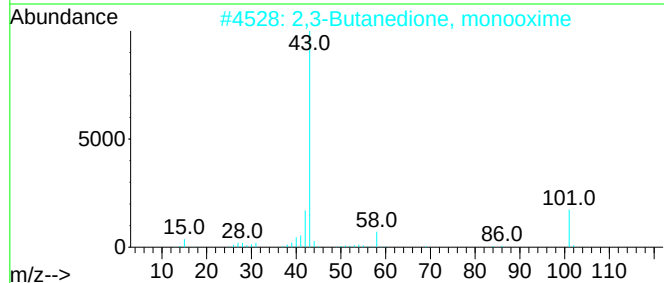
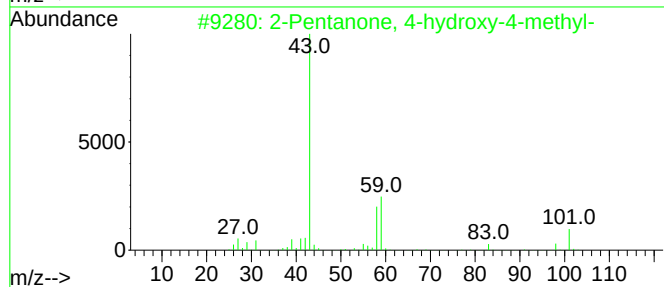
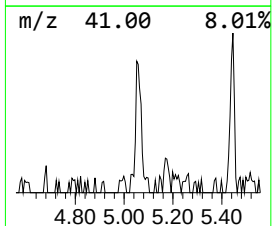
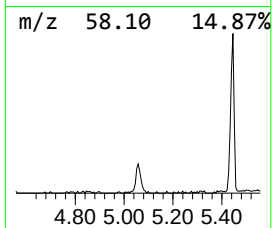
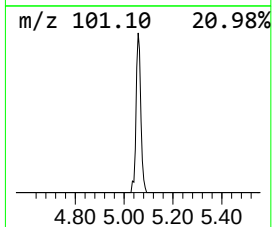
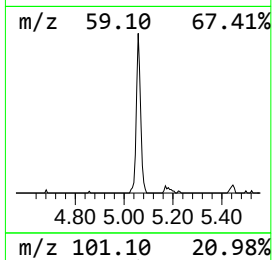
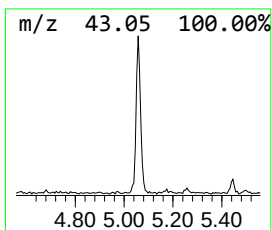
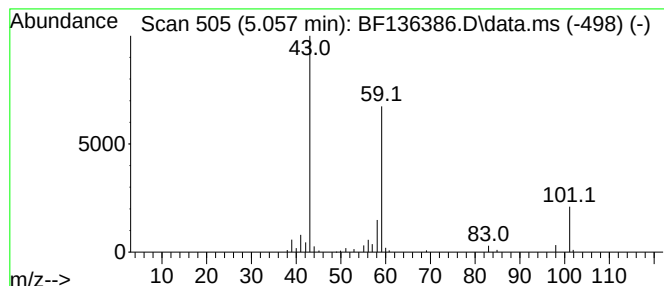
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	2.30 ng	81768	1,4-Dichlorobenzene-d4	6.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		3-Octanol	130	C8H18O	000589-98-0	33
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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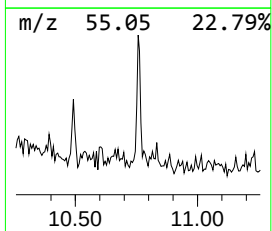
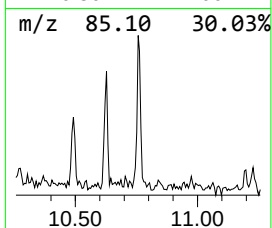
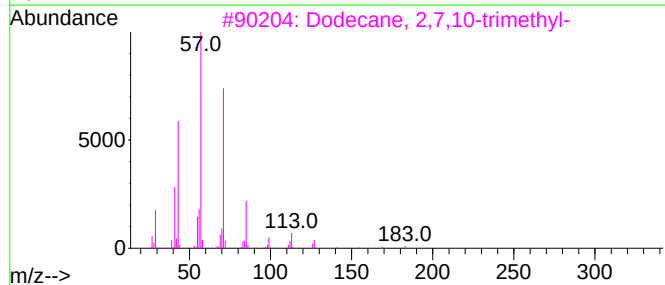
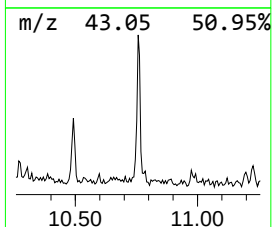
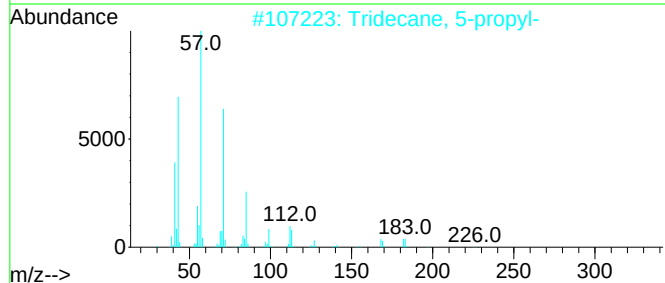
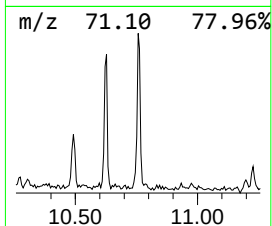
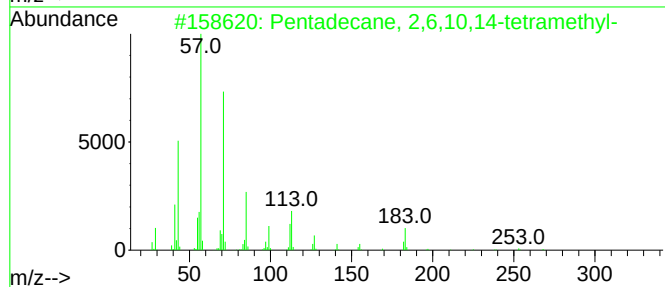
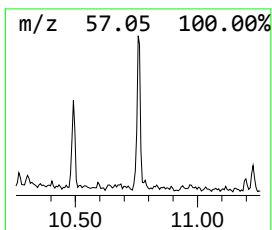
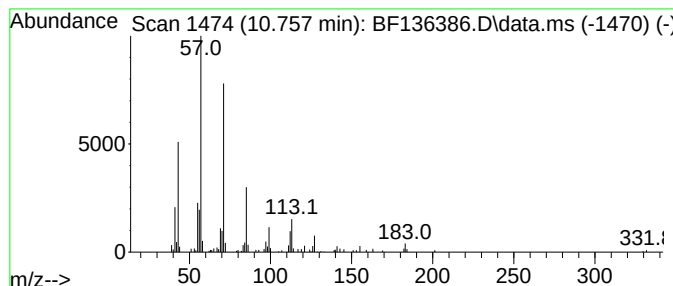
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Peak Number 3 Pentadecane, 2,6,10,14-tetr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	2.03 ng	80710	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	91
2			Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
3			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
4			Undecane, 6-ethyl-	184	C13H28	017312-60-6	74
5			Tridecane, 4-methyl-	198	C14H30	026730-12-1	72



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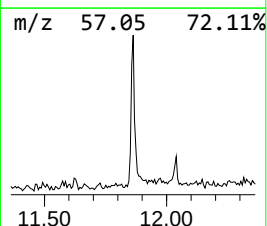
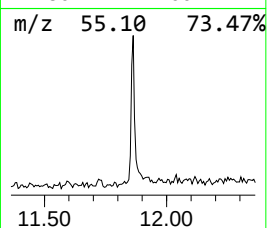
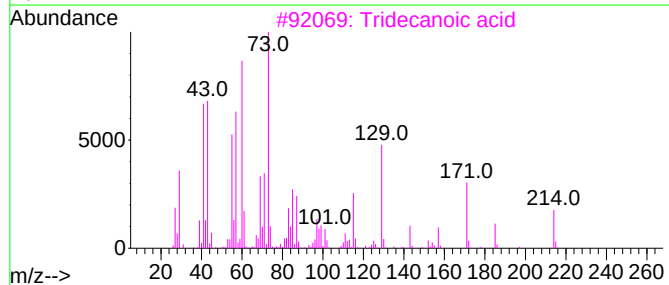
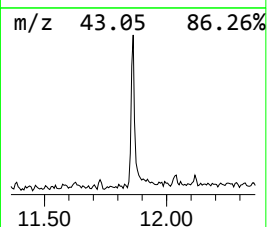
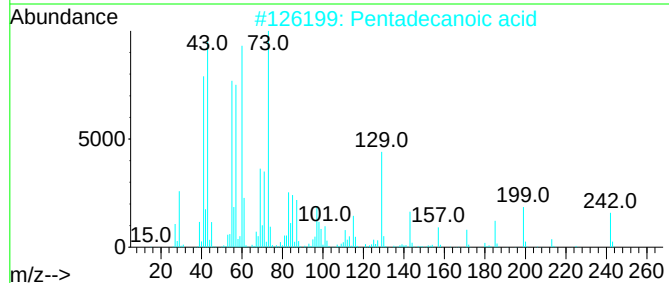
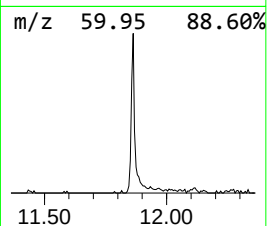
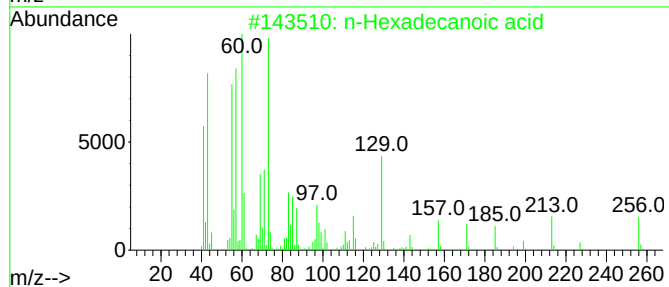
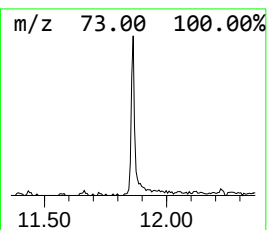
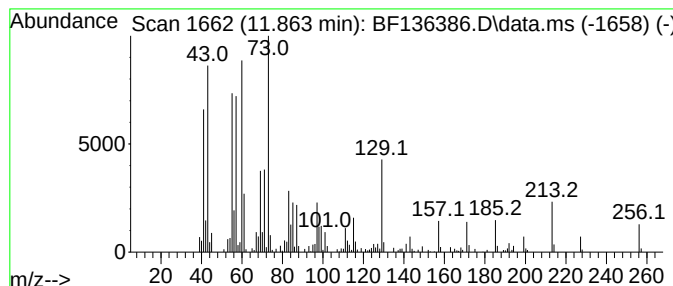
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	5.63 ng	223607	Phenanthrene-d10	11.328

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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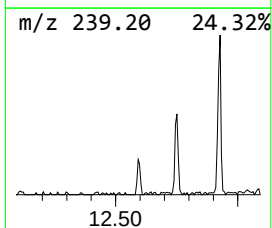
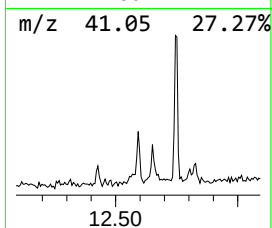
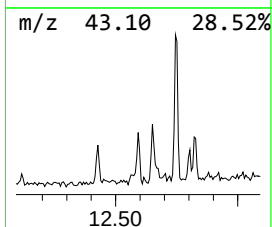
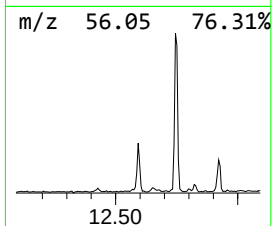
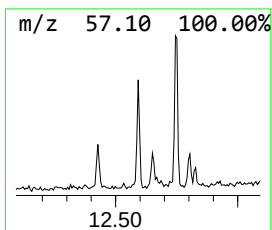
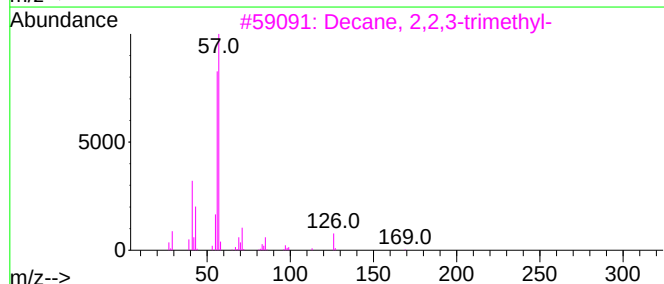
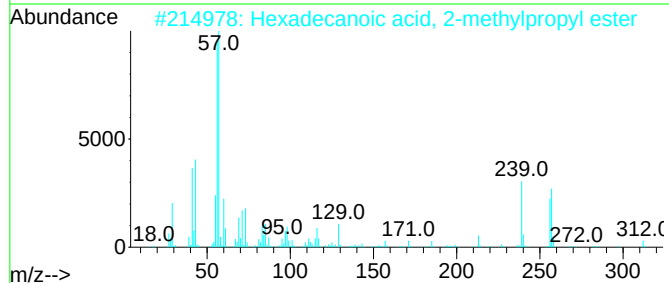
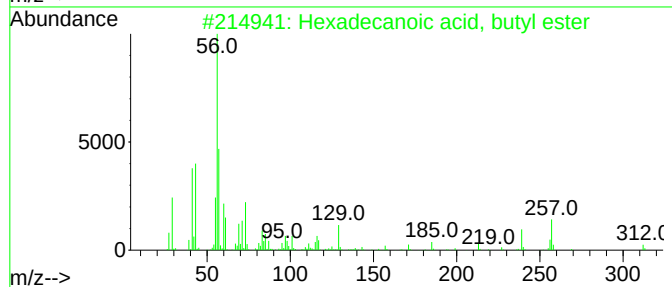
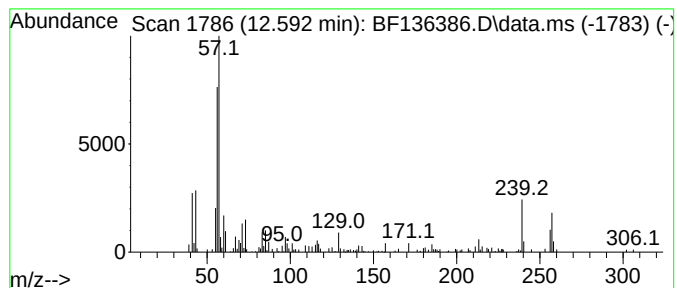
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	2.09 ng	83187	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	81
2			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	80
3			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	38
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	37



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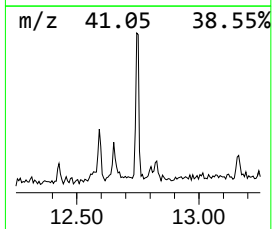
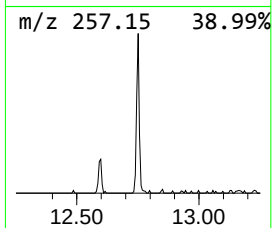
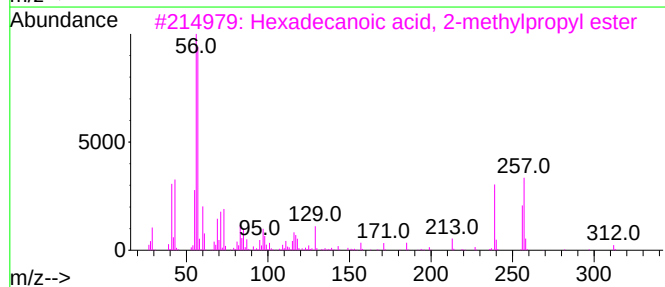
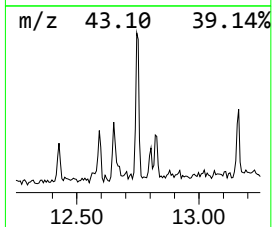
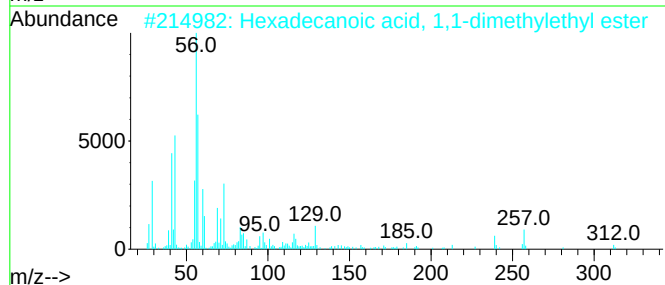
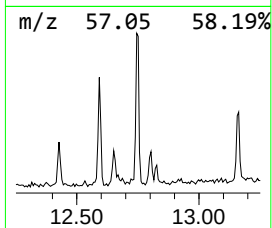
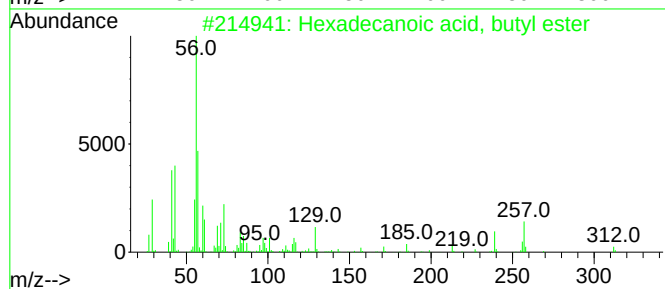
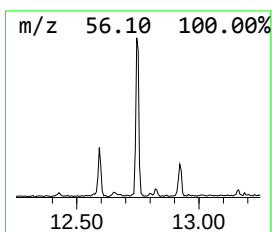
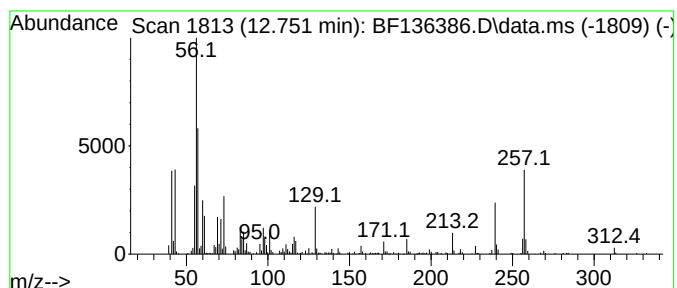
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	6.55 ng	233248	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	98
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	95
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	64
4			Nipecotic acid	129	C6H11NO2	000498-95-3	43
5			Butyl 15-methylhexadecanoate	326	C21H42O2	1000336-52-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136386.D
Acq On : 04 Dec 2023 17:27
Operator : CG\JU
Sample : 05434-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

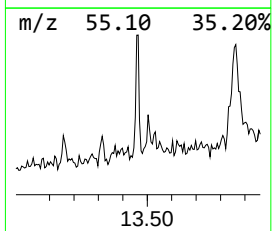
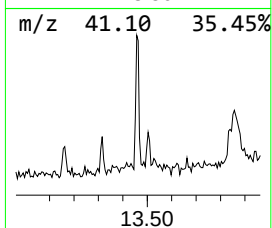
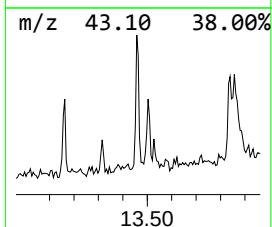
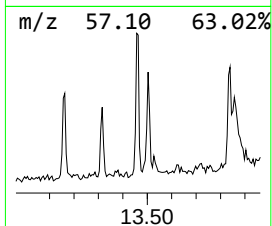
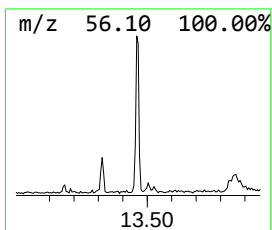
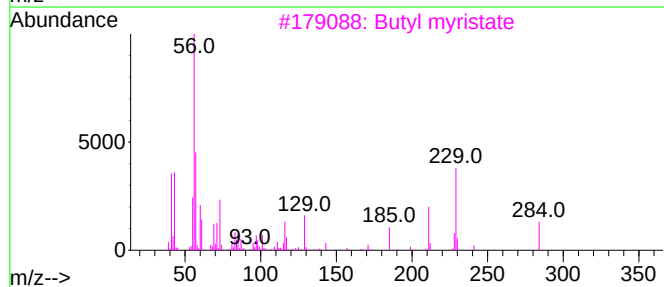
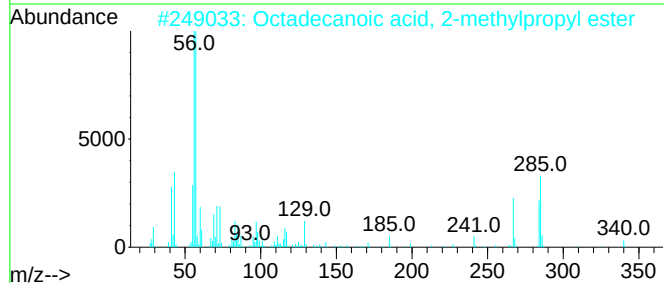
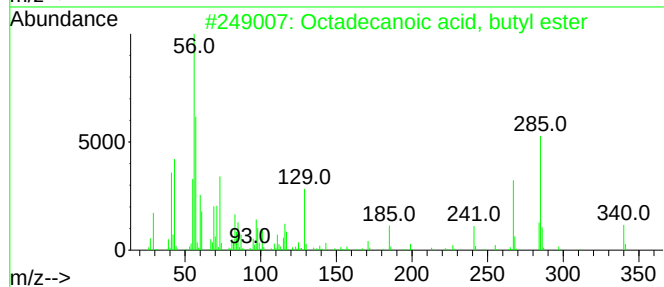
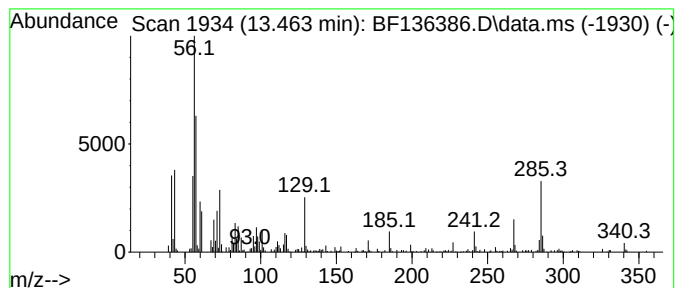
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.463	4.83 ng	172043	Chrysene-d12	13.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	99
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	90
3	Butyl myristate	284	C18H36O2	000110-36-1	52
4	Docosanoic acid, isobutyl ester	396	C26H52O2	1000405-17-1	43
5	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136386.D
Acq On : 04 Dec 2023 17:27
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Sample : 05434-15
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Instrument :
BNA_F
ClientSampleId :
COMP-8

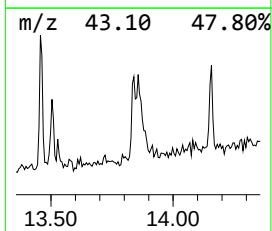
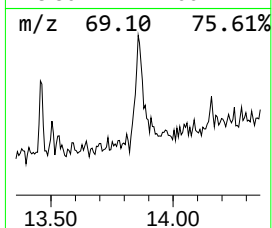
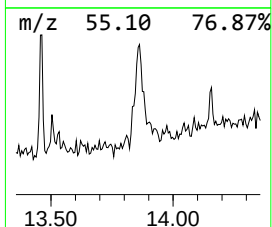
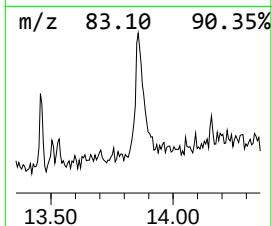
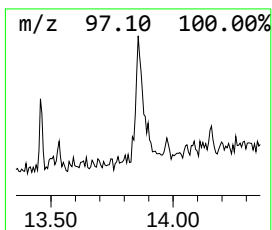
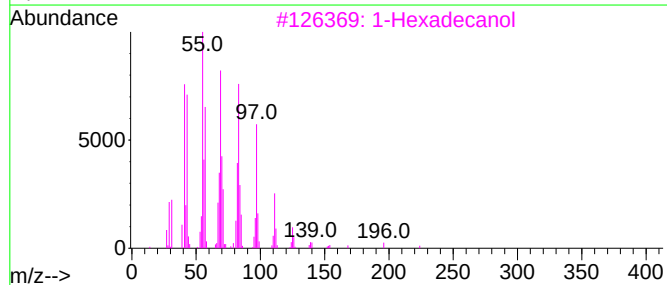
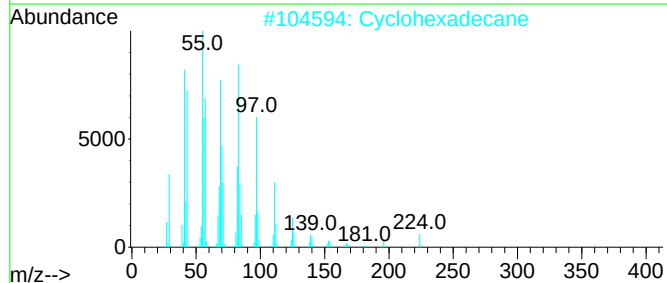
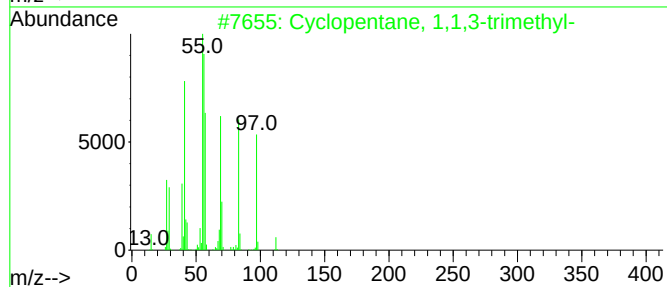
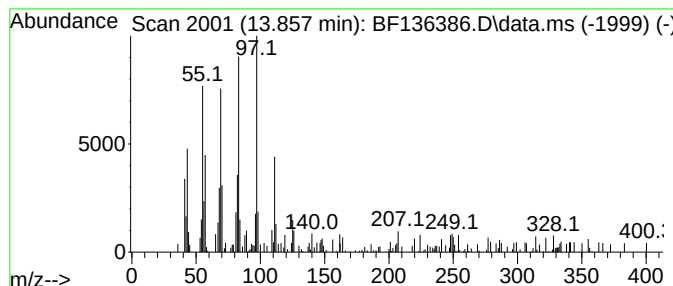
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopentane, 1,1,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	3.51 ng	125238	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	76
2			Cyclohexadecane	224	C16H32	000295-65-8	58
3			1-Hexadecanol	242	C16H34O	036653-82-4	52
4			3-Heptene, 4-propyl-	140	C10H20	004485-13-6	49
5			2,6-Dodecadien-1-ol, 3,7,11-trim...	224	C15H28O	020576-56-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136386.D
Acq On : 04 Dec 2023 17:27
Operator : CG\JU
Sample : 05434-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

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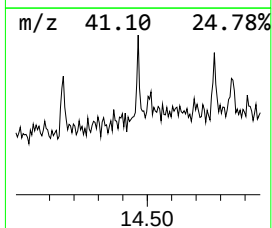
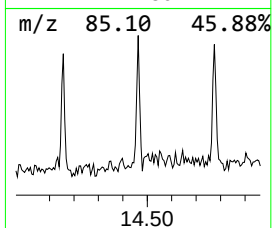
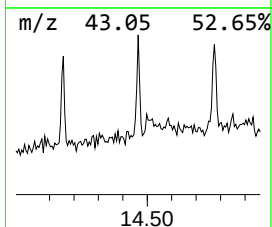
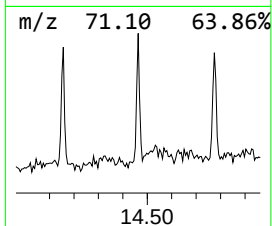
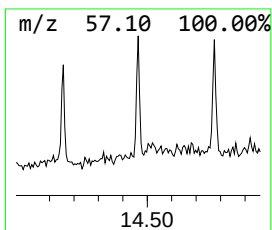
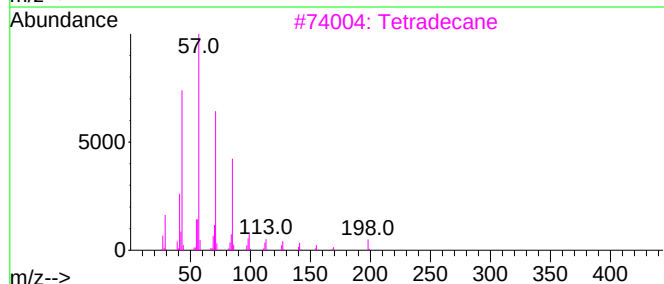
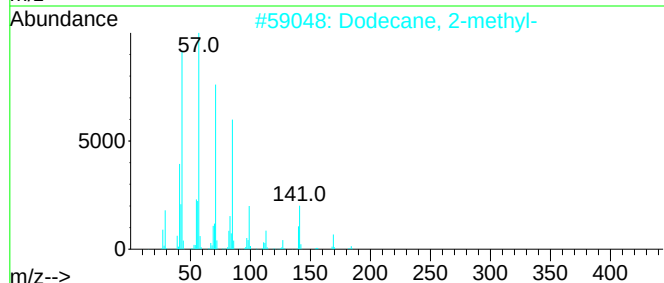
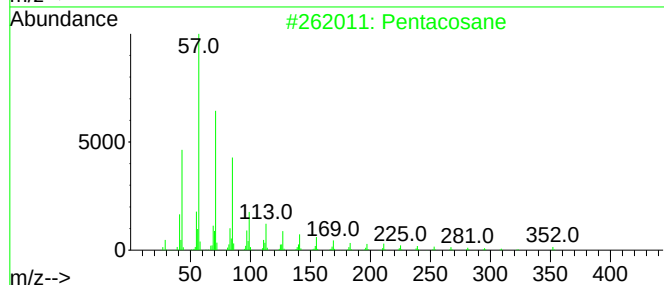
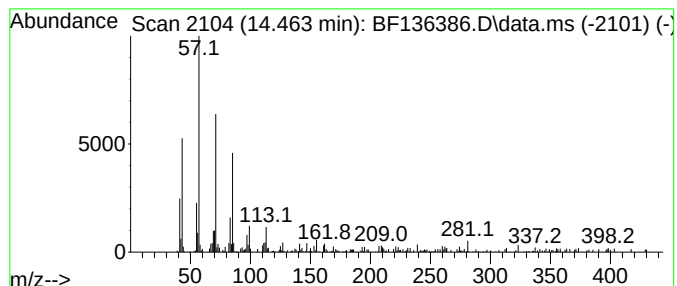
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	2.26 ng	80399	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	92
2			Dodecane, 2-methyl-	184	C13H28	001560-97-0	76
3			Tetradecane	198	C14H30	000629-59-4	68
4			Heptacosane	380	C27H56	000593-49-7	68
5			Pentadecane	212	C15H32	000629-62-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136386.D
Acq On : 04 Dec 2023 17:27
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Sample : 05434-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

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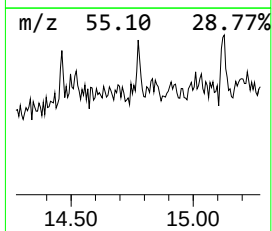
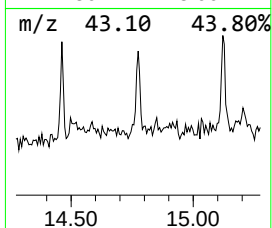
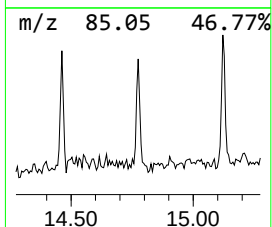
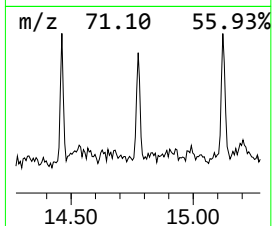
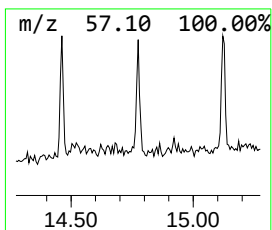
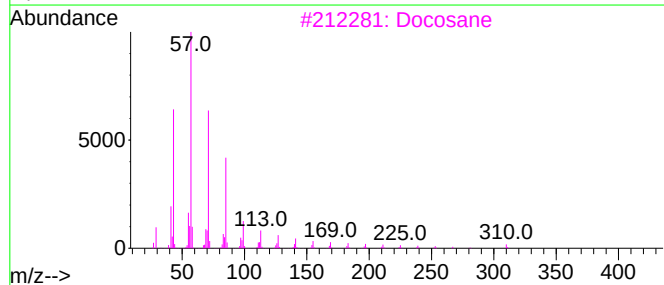
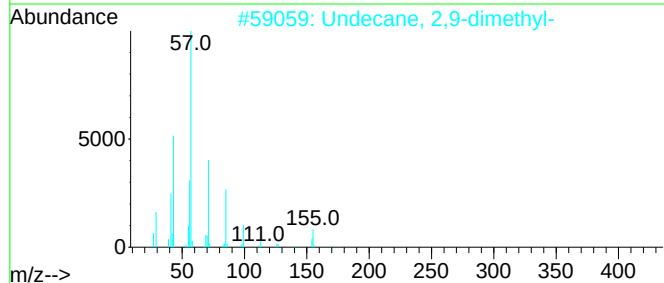
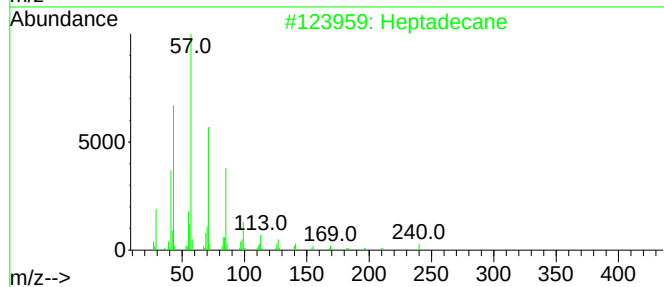
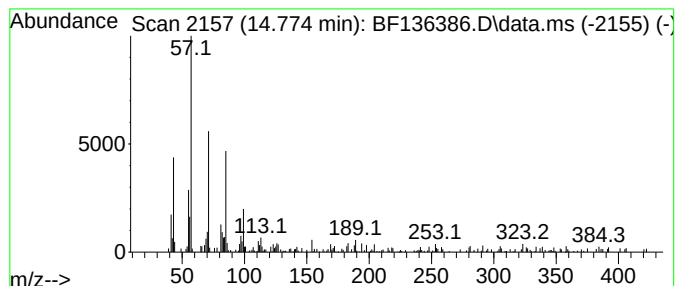
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	2.49 ng	63778	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	76
2		Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	72
3		Docosane	310	C22H46	000629-97-0	64
4		Octadecane	254	C18H38	000593-45-3	64
5		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136386.D
Acq On : 04 Dec 2023 17:27
Operator : CG\JU
Sample : 05434-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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2-Pentanone, 4-...	5.057	2.3	ng	81768	1	6.804	710483	20.0
Pentadecane, 2,...	10.757	2.0	ng	80710	4	11.328	794866	20.0
n-Hexadecanoic ...	11.863	5.6	ng	223607	4	11.328	794866	20.0
Hexadecanoic ac...	12.592	2.1	ng	83187	4	11.328	794866	20.0
Hexadecanoic ac...	12.751	6.5	ng	233248	5	13.980	712669	20.0
Octadecanoic ac...	13.463	4.8	ng	172043	5	13.980	712669	20.0
Cyclopentane, 1...	13.857	3.5	ng	125238	5	13.980	712669	20.0
Pentacosane	14.463	2.3	ng	80399	5	13.980	712669	20.0
Heptadecane	14.774	2.5	ng	63778	6	15.463	512301	20.0