LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138541.D
Acq On : 12 Jul 2024 12:23
Operator : CG\JU
Sample : PB162009BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB162009BL

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: BF138541.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	24	32	38	rVB	89872	123427	2.49%	0.402%
2	5.122	511	516	527	rVB	198231	309864	6.24%	1.010%
3	5.510	576	582	585	rBV	3802989	3874978	78.07%	12.632%
4	6.504	745	751	754	rBV	3258524	4040483	81.40%	13.172%
5	6.863	808	812	816	rBV	1024825	818363	16.49%	2.668%
6	7.434	902	909	911	rBV	2219429	2711168	54.62%	8.838%
7	8.145	1024	1030	1033	rBV	1243629	1110010	22.36%	3.619%
8	9.222	1206	1213	1216	rBV	4314115	4780090	96.30%	15.583%
9	9.898	1322	1328	1331	rBV	1555060	1315102	26.49%	4.287%
10	10.692	1456	1463	1466	rBV	3036874	3001155	60.46%	9.784%
11	11.386	1577	1581	1584	rBV	1680233	1368308	27.57%	4.461%
12	12.633	1789	1793	1796	rBV	85823	64156	1.29%	0.209%
13	12.786	1815	1819	1822	rBV	248568	191975	3.87%	0.626%
14	12.974	1846	1851	1854	rBV	4714630	4963755	100.00%	16.182%
15	13.492	1934	1939	1942	rBV	159271	137301	2.77%	0.448%
16	14.021	2025	2029	2039	rBV	1095716	953194	19.20%	3.107%
17	15.486	2273	2278	2290	rBV	527094	724196	14.59%	2.361%
18	17.039	2528	2542	2555	rBV6	43324	187353	3.77%	0.611%

Sum of corrected areas: 30674878

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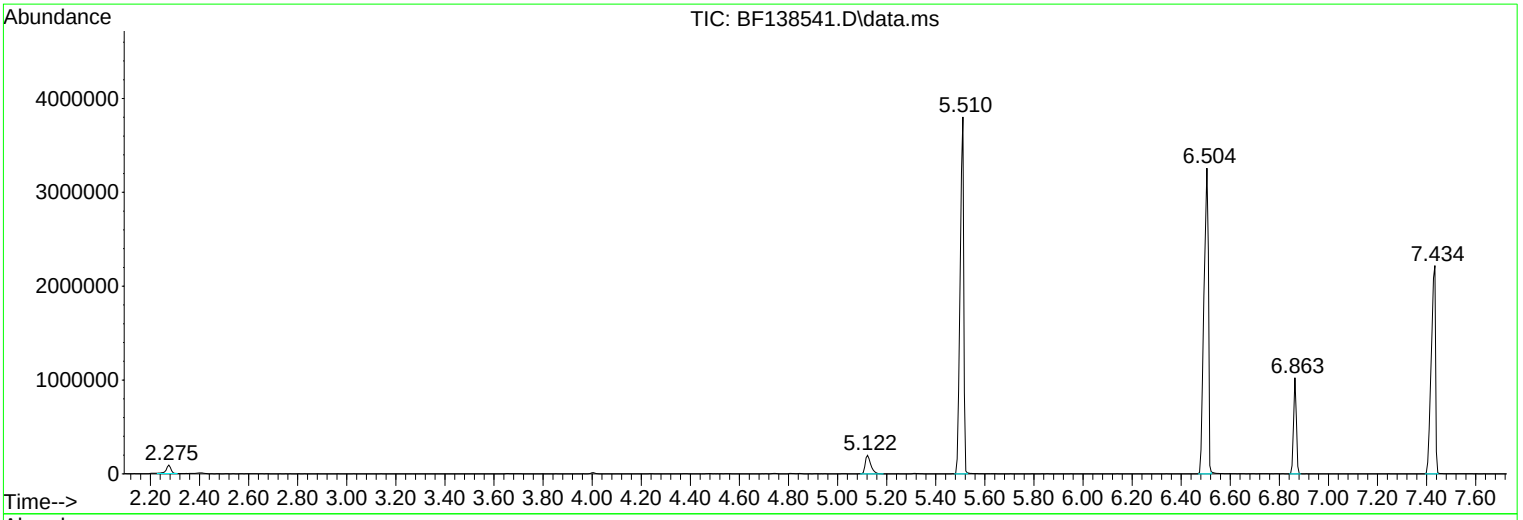
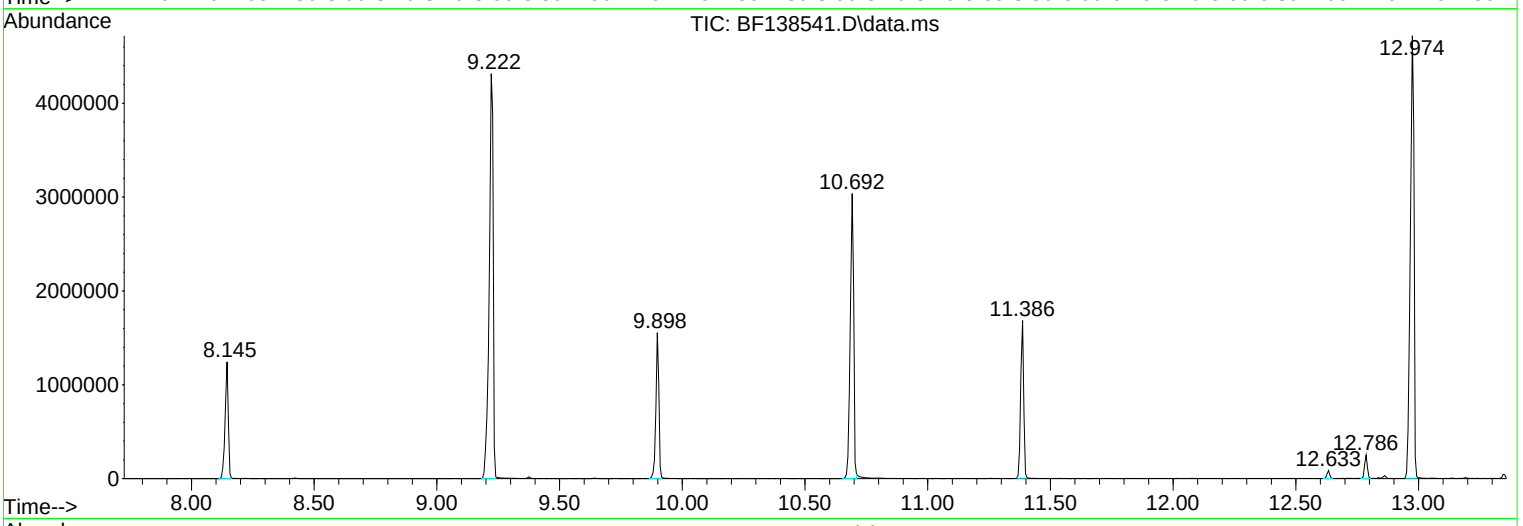
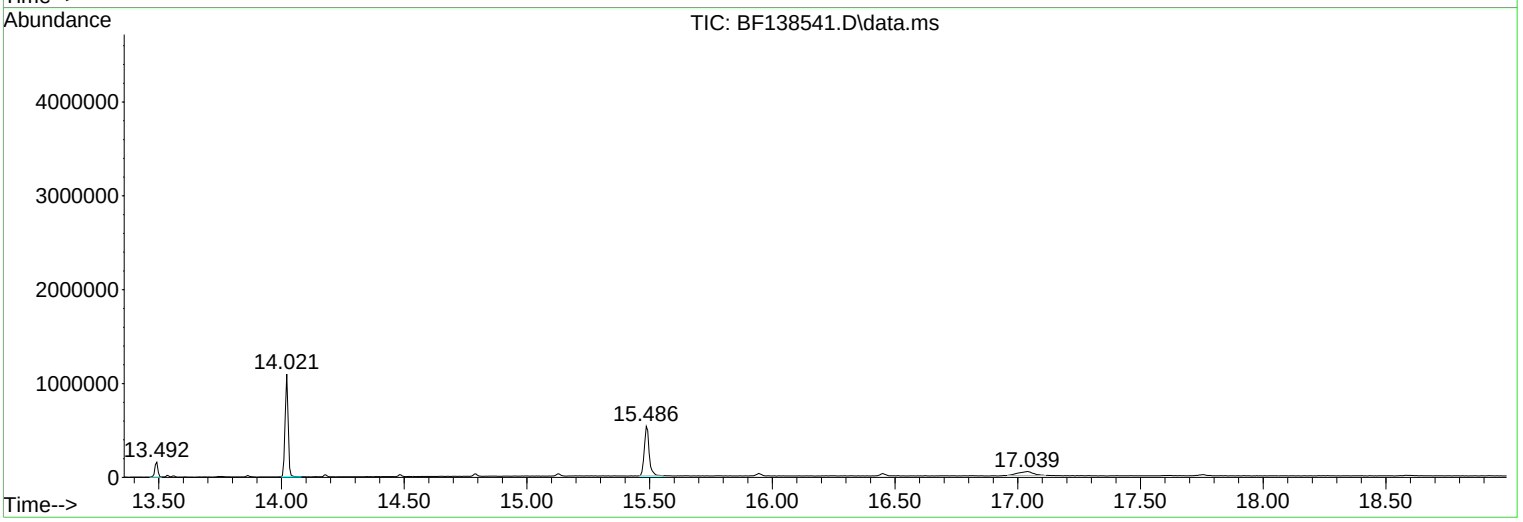
Instrument :
BNA_F
ClientSampleId :
PB162009BL

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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Data File : BF138541.D
Acq On : 12 Jul 2024 12:23
Operator : CG\JU
Sample : PB162009BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB162009BL

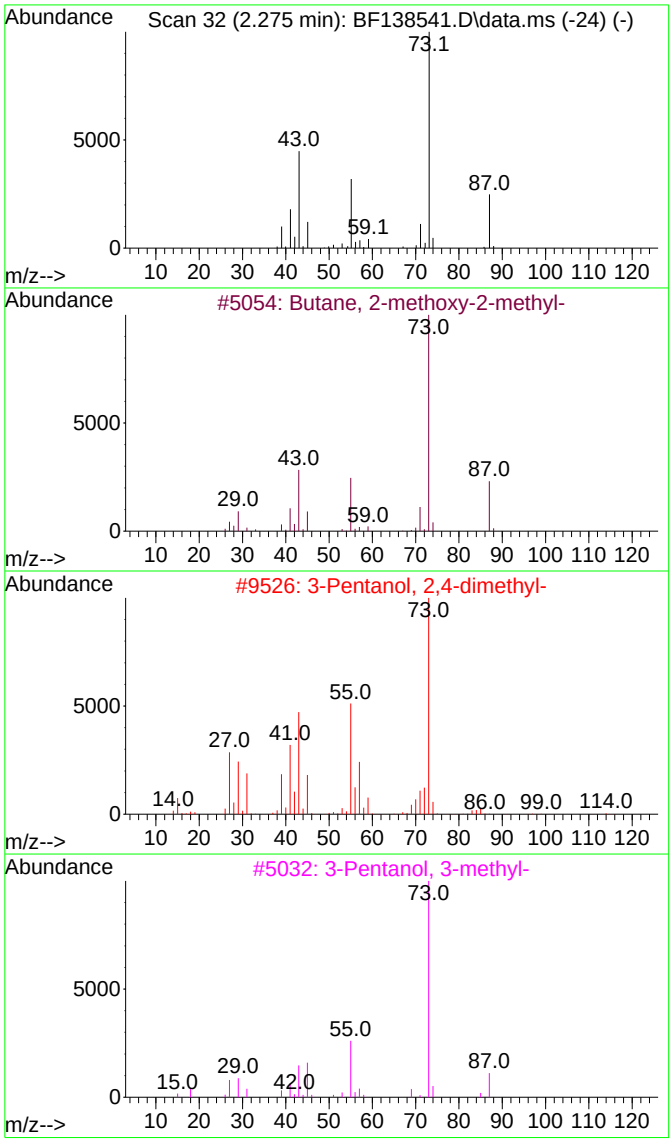
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

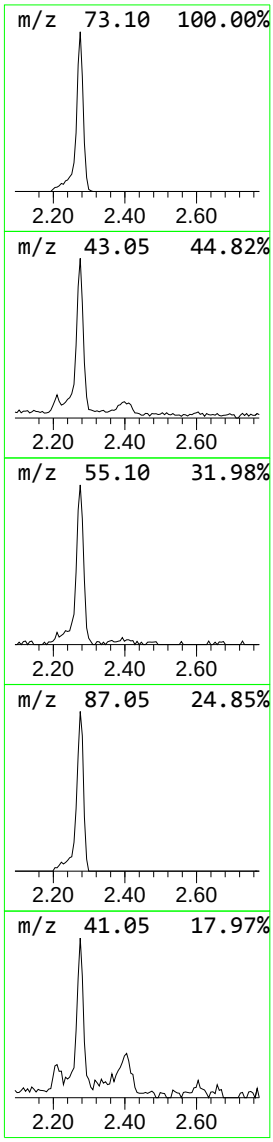
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	3.02 ng	123427	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	74
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	28
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Operator : CG\JU
Sample : PB162009BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB162009BL

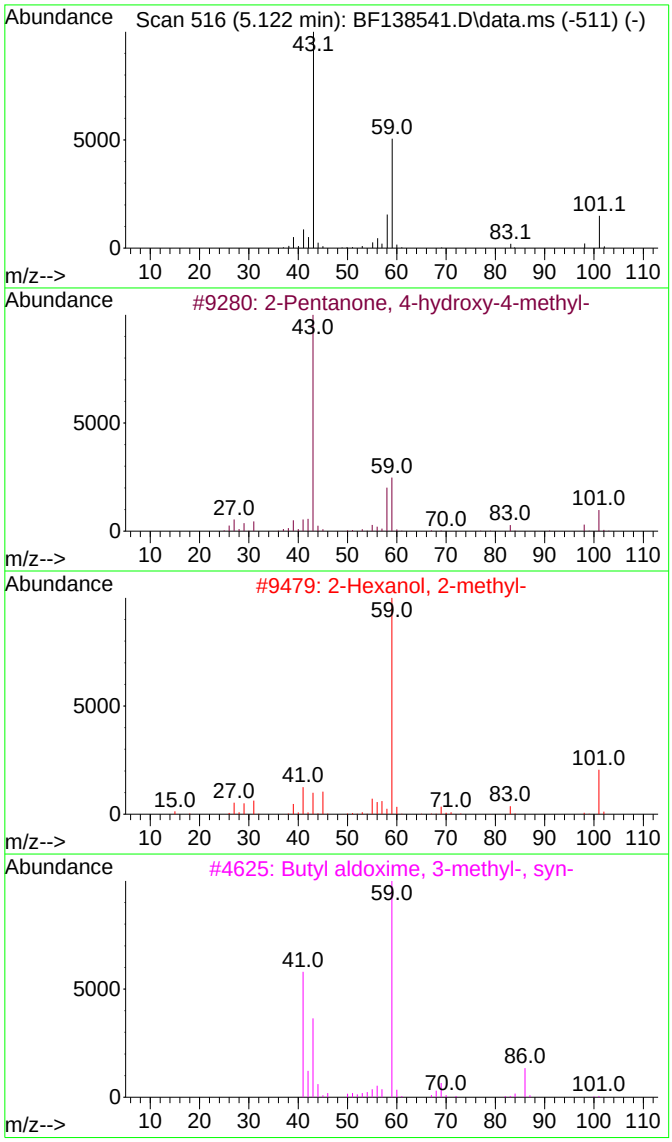
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

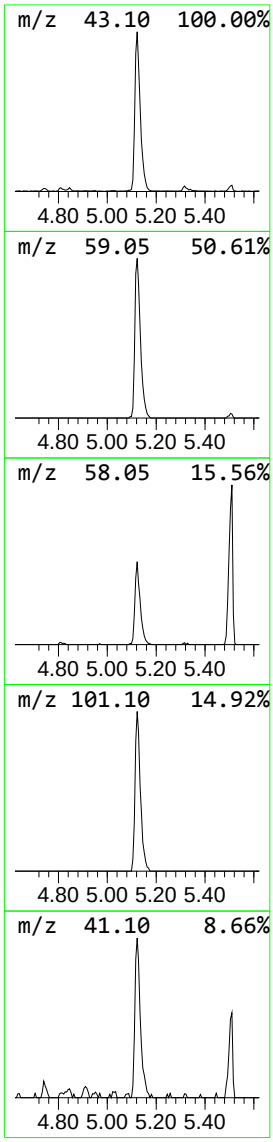
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	7.57 ng	309864	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	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Operator : CG\JU
Sample : PB162009BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB162009BL

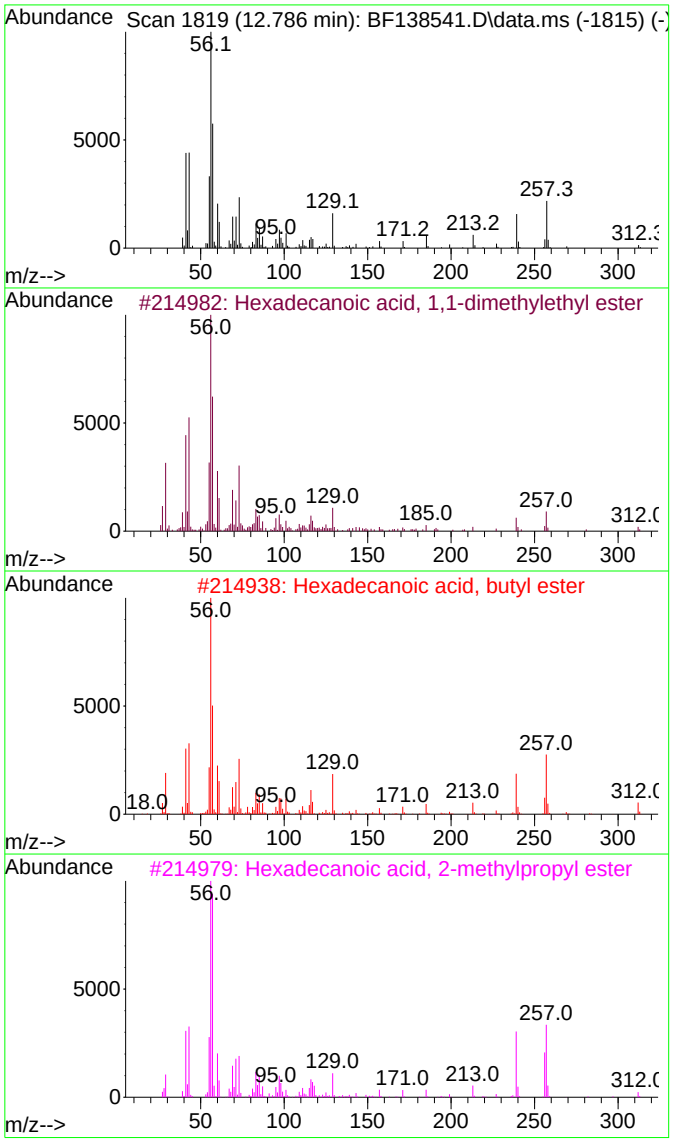
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

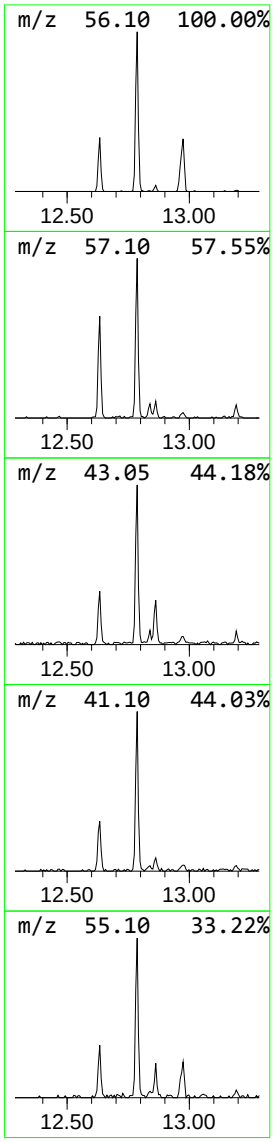
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexadecanoic acid, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	4.03 ng	191975	Chrysene-d12	14.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	98
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	87
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27
5	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	27





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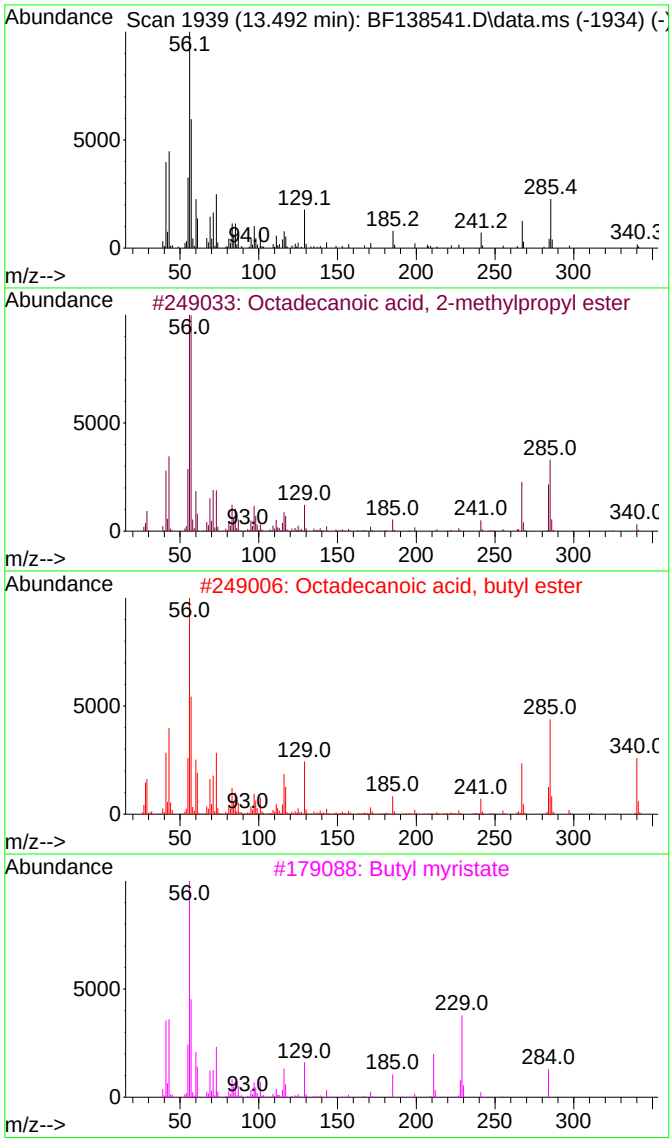
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

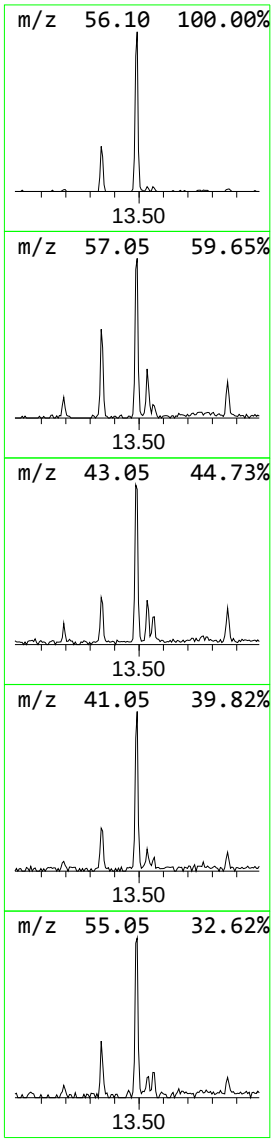
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octadecanoic acid, 2-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	2.88 ng	137301	Chrysene-d12	14.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	90
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	74
3	Butyl myristate	284	C18H36O2	000110-36-1	64
4	Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32
5	Docosanoic acid, isobutyl ester	396	C26H52O2	1000405-17-1	30





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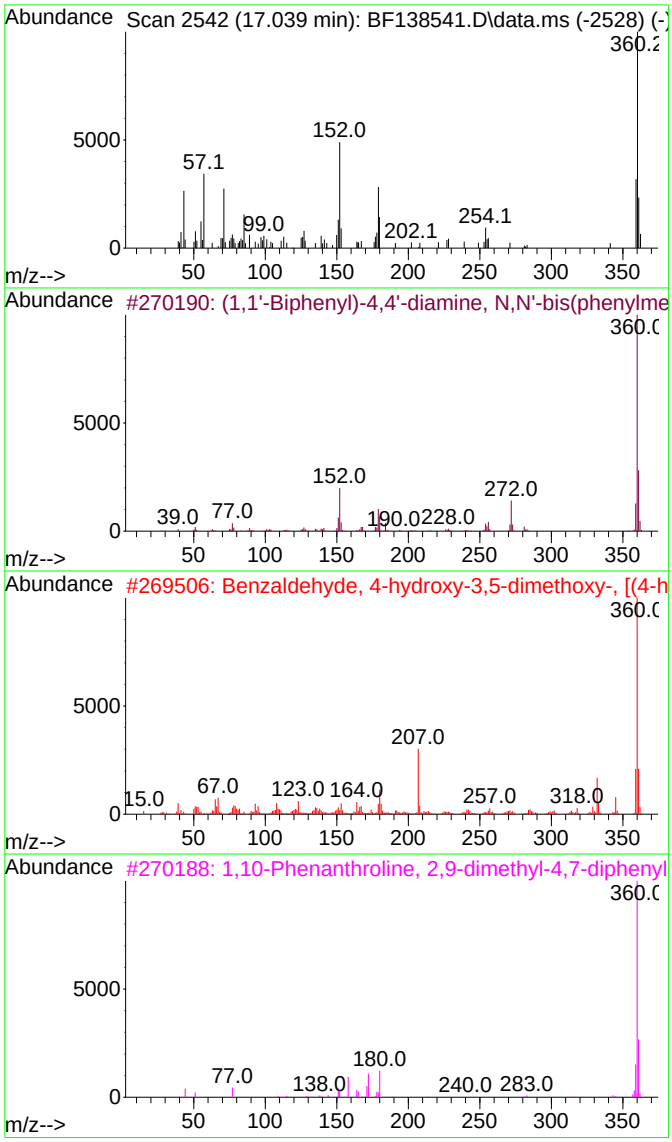
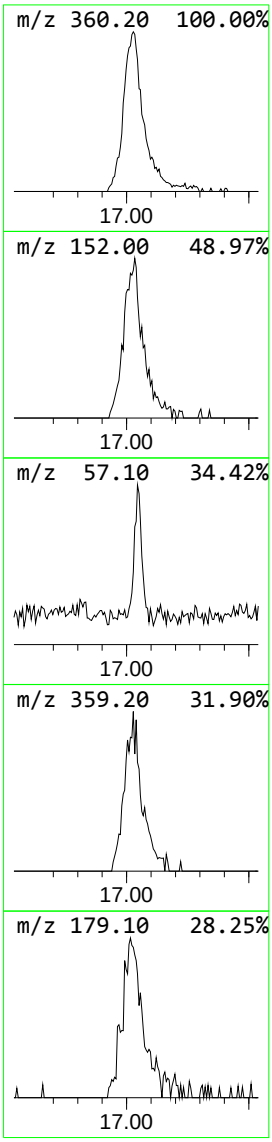
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.039	5.17 ng	187353	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	91
2	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
3	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43
4	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	43
5	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	38





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.275	3.0	ng	123427	1	6.863	818363	20.0
2-Pentanone, 4-...	5.122	7.6	ng	309864	1	6.863	818363	20.0
Hexadecanoic ac...	12.786	4.0	ng	191975	5	14.022	953194	20.0
Octadecanoic ac...	13.492	2.9	ng	137301	5	14.022	953194	20.0
(1,1'-Biphenyl)...	17.039	5.2	ng	187353	6	15.486	724196	20.0