LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF130986.D
Acq On : 04 Nov 2022 11:44
Operator : CG\JU
Sample : PB148687BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148687BL

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130986.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	19	32	38	rVB	103493	148271	4.53%	0.720%
2	2.387	45	51	57	rBV	47636	63544	1.94%	0.309%
3	5.157	517	522	532	rVB	304267	420630	12.86%	2.044%
4	5.540	582	587	590	rBV	2662283	2743217	83.85%	13.327%
5	6.539	751	757	760	rBV	2520124	2780360	84.99%	13.508%
6	6.910	817	820	824	rVB	714868	622856	19.04%	3.026%
7	7.481	911	917	920	rBV	1647009	1815271	55.49%	8.819%
8	8.198	1034	1039	1042	rBV	894627	816433	24.96%	3.966%
9	9.280	1216	1223	1226	rBV	3192516	3271474	100.00%	15.894%
10	9.963	1333	1339	1342	rBV	988751	939144	28.71%	4.563%
11	10.757	1467	1474	1477	rBV	1829181	1756961	53.71%	8.536%
12	11.451	1588	1592	1596	rBV	804678	754669	23.07%	3.666%
13	13.051	1859	1864	1867	rBV	3107935	2885966	88.22%	14.021%
14	14.104	2039	2043	2047	rBV	737518	631948	19.32%	3.070%
15	14.198	2053	2059	2064	rBV	68884	92844	2.84%	0.451%
16	14.880	2172	2175	2180	rVB	31618	33801	1.03%	0.164%
17	15.233	2232	2235	2240	rVB	41981	45063	1.38%	0.219%
18	15.615	2294	2300	2310	rBV	335567	517308	15.81%	2.513%
19	16.092	2376	2381	2385	rBV2	37919	55824	1.71%	0.271%
20	16.621	2467	2471	2476	rVB2	45168	70880	2.17%	0.344%
21	17.251	2572	2578	2586	rVB2	33145	72767	2.22%	0.354%
22	17.998	2700	2705	2711	rVB3	20697	44162	1.35%	0.215%

Sum of corrected areas: 20583393

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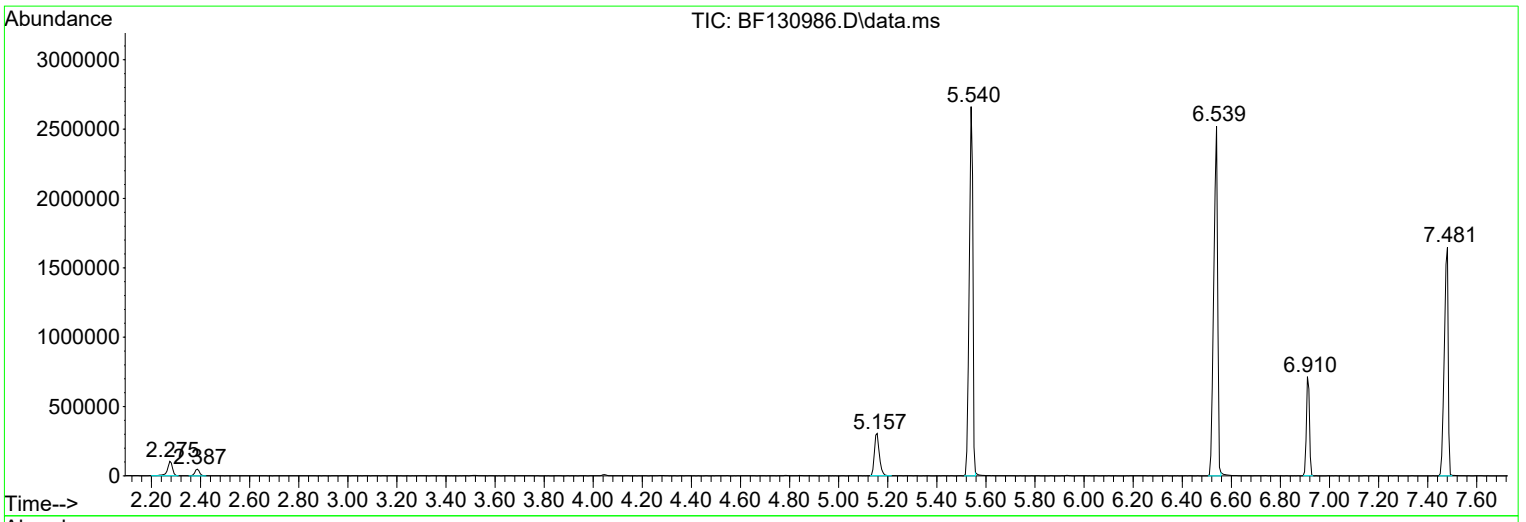
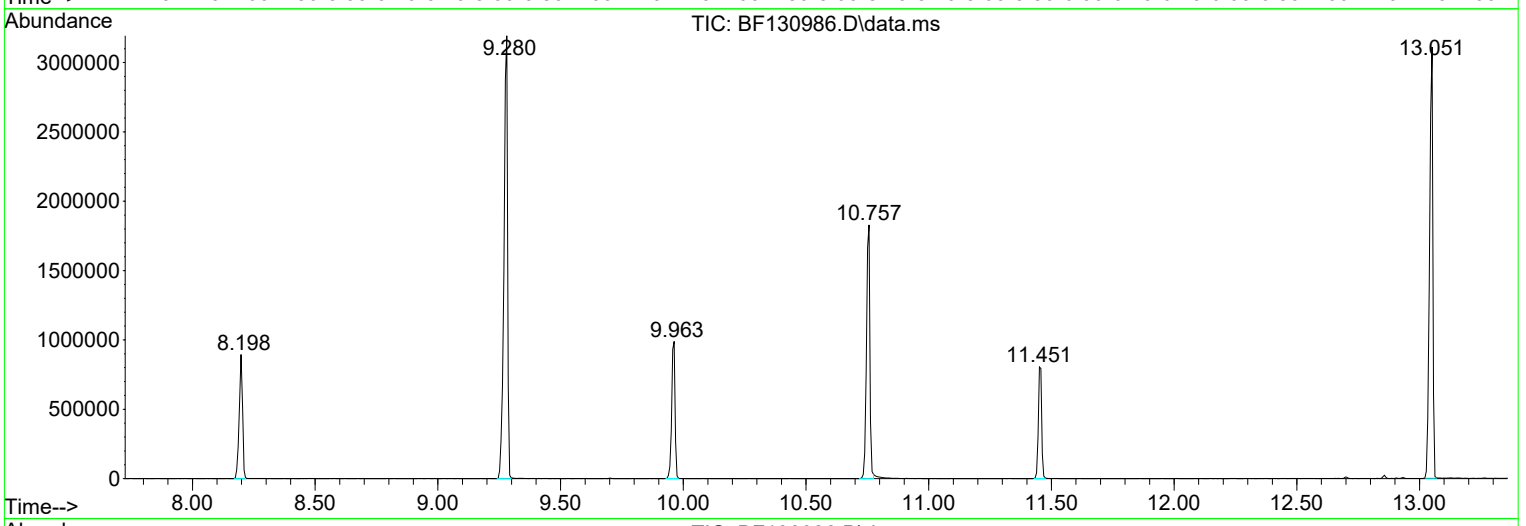
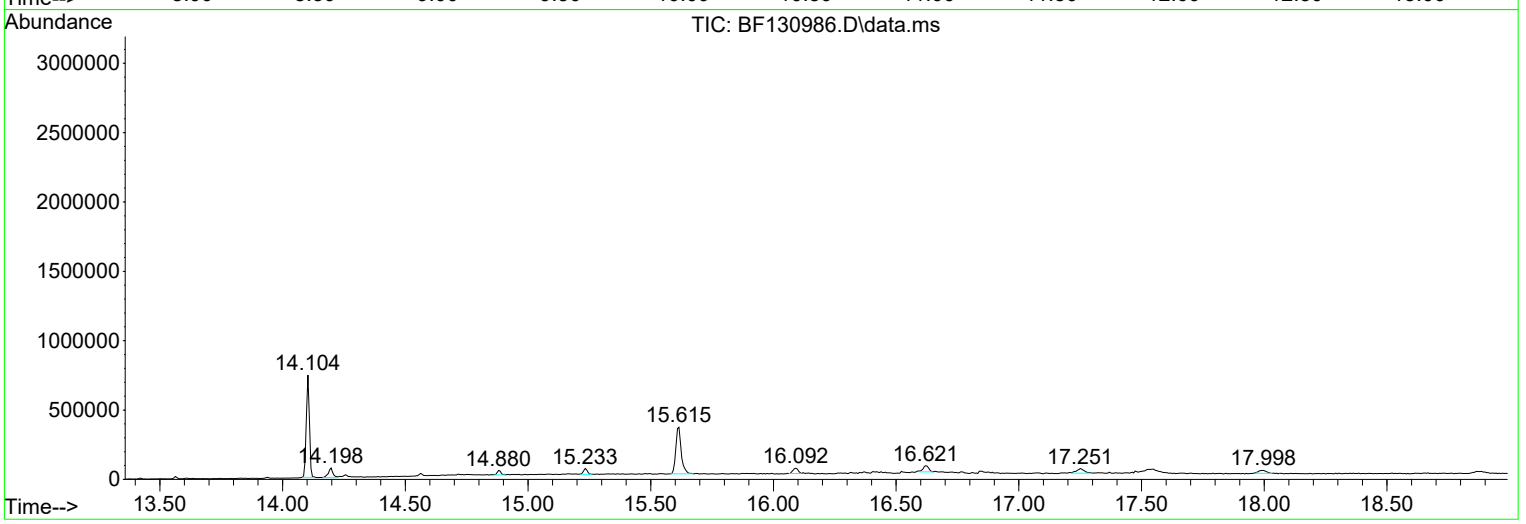
ClientSampleId :
PB148687BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

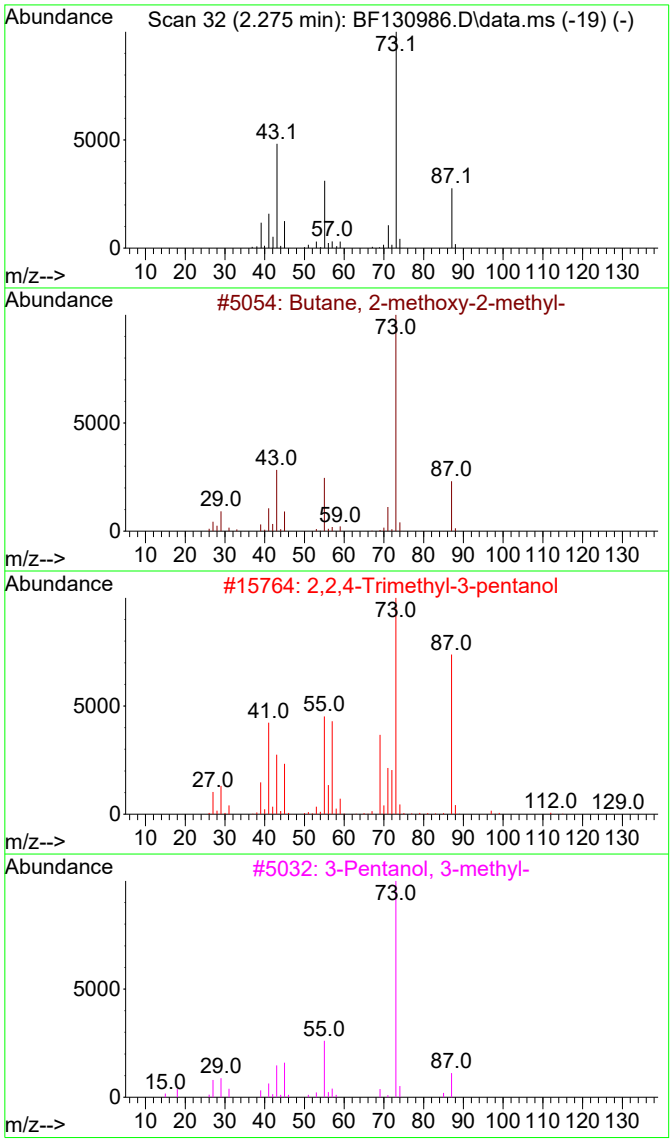
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

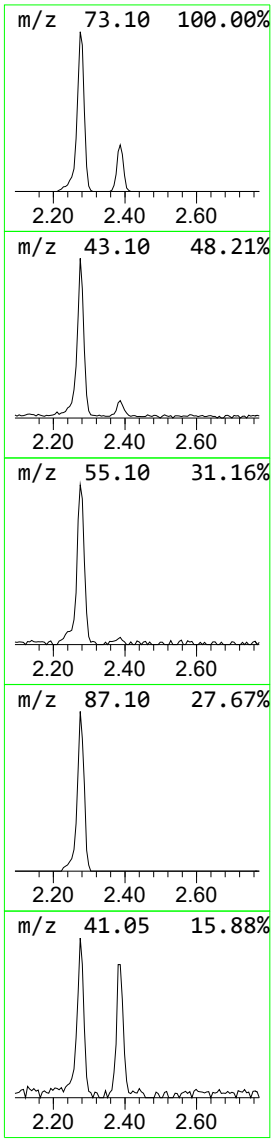
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	4.76 ng	148271	1,4-Dichlorobenzene-d4	6.910

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	39
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





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Instrument :
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ClientSampleId :
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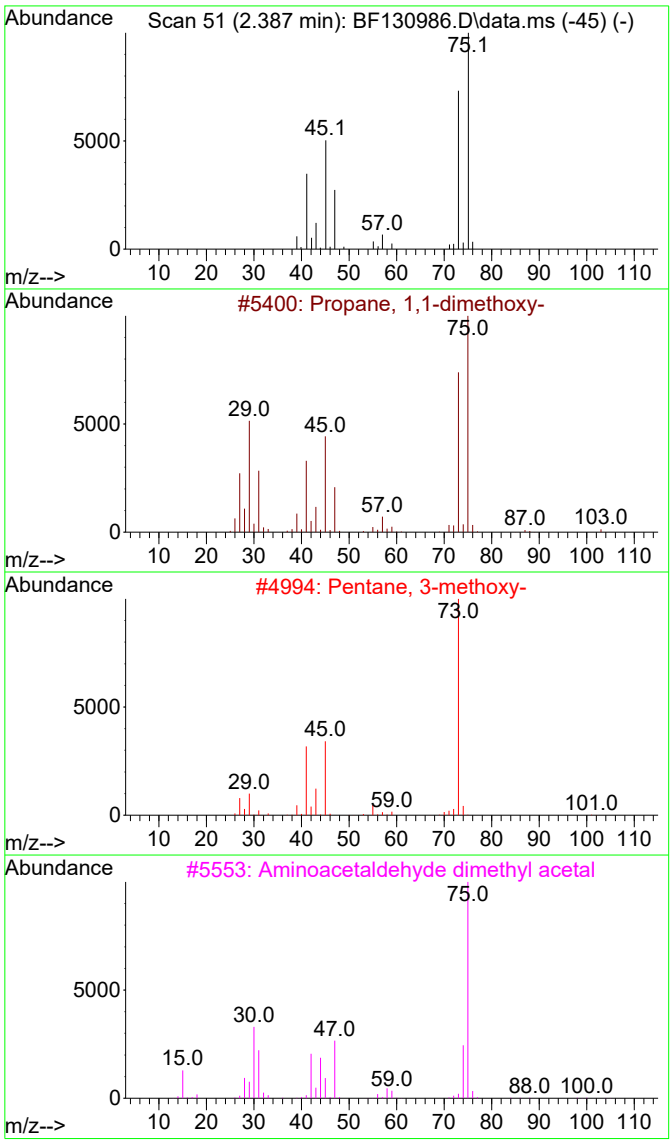
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

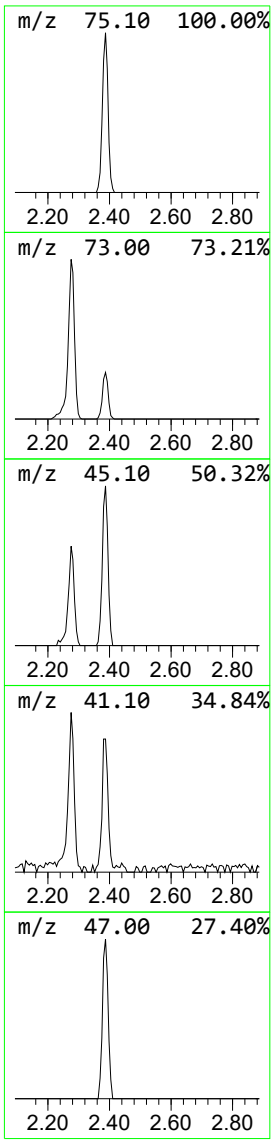
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.387	2.04 ng	63544	1,4-Dichlorobenzene-d4	6.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
4	Methane, trimethoxy-	106	C4H10O3	000149-73-5	9
5	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9





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Sample : PB148687BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB148687BL

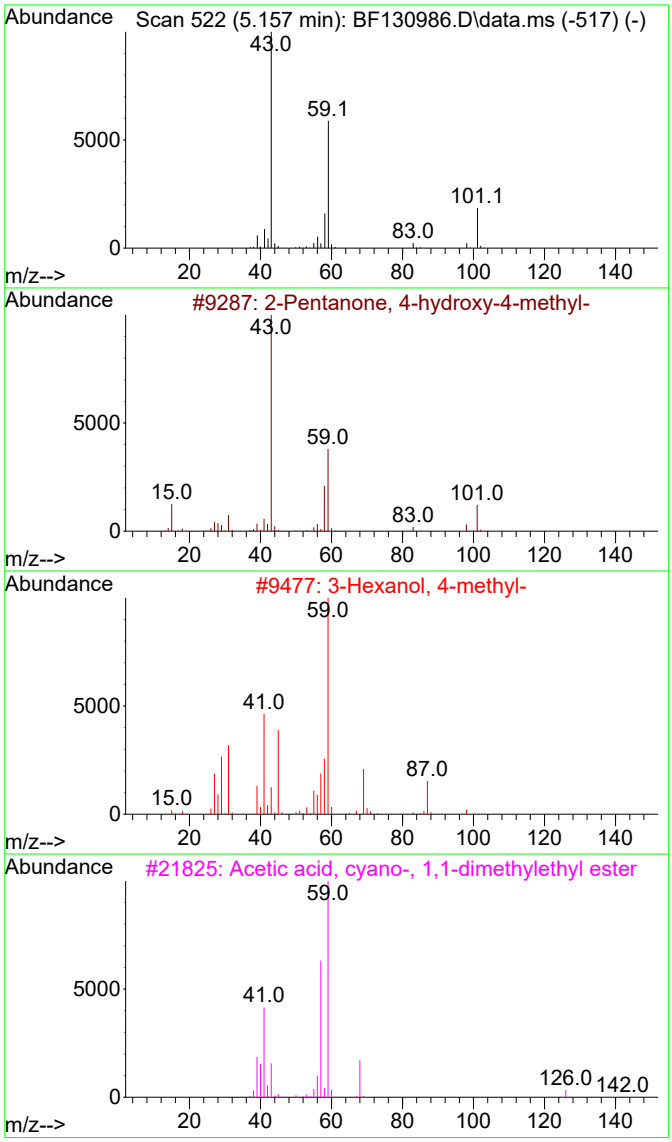
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

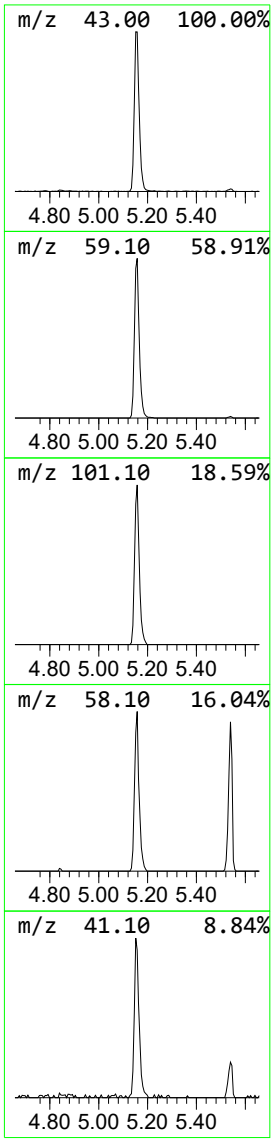
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	13.51 ng	420630	1,4-Dichlorobenzene-d4	6.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

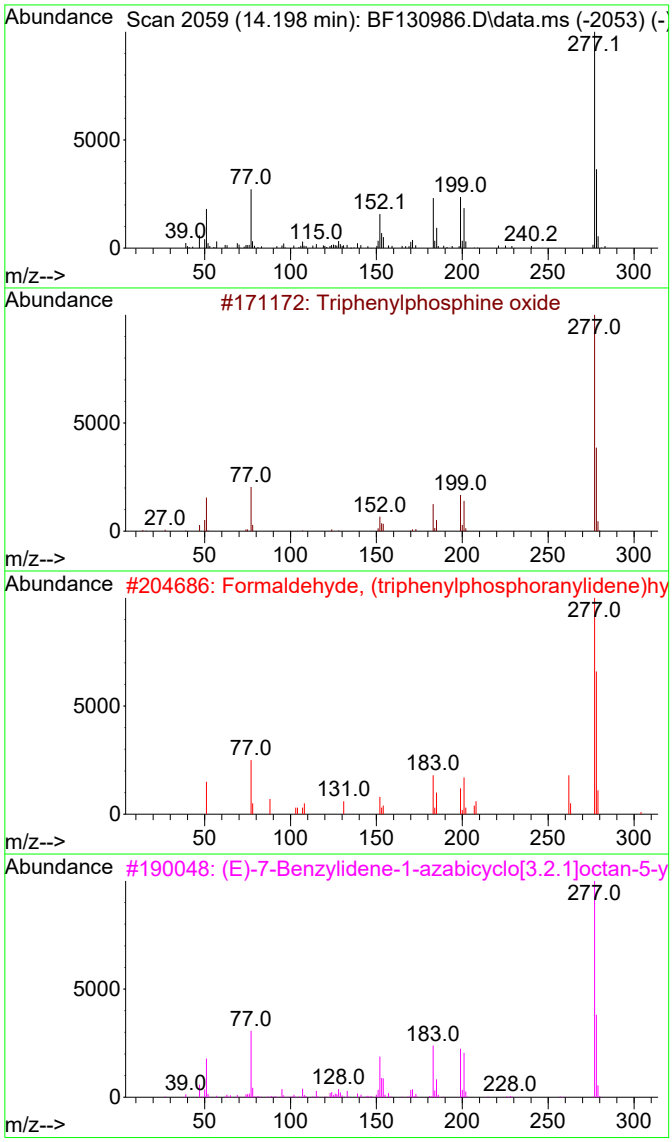
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

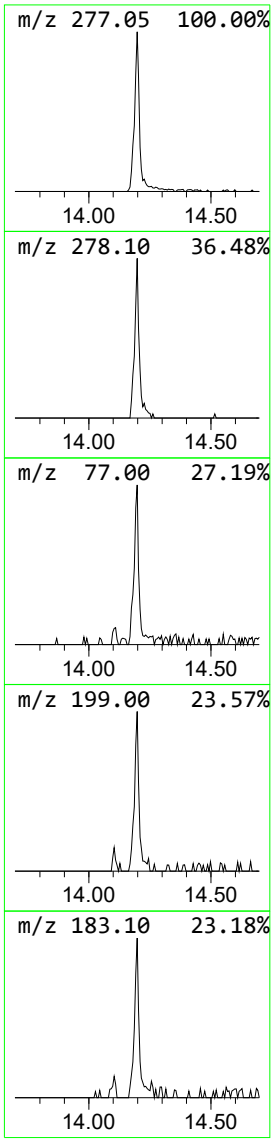
****

Peak Number 4 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	2.94 ng	92844	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	50
4	Butylaldehyde, 4-benzyloxy-4-[2,...	278	C16H22O4	149180-87-0	43
5	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43





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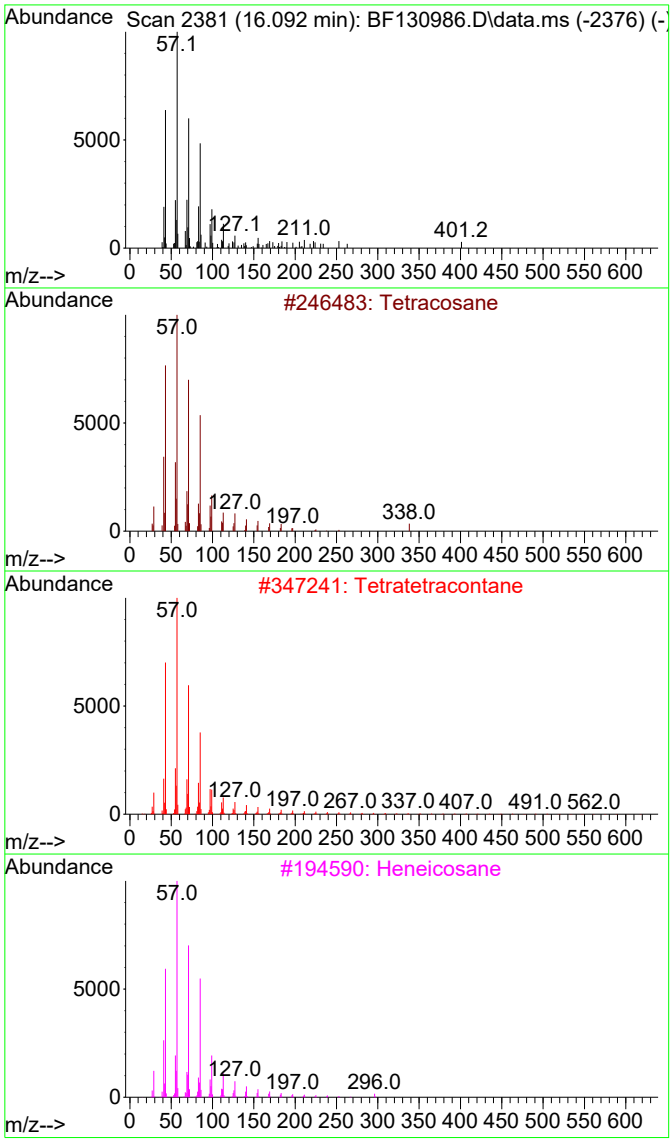
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

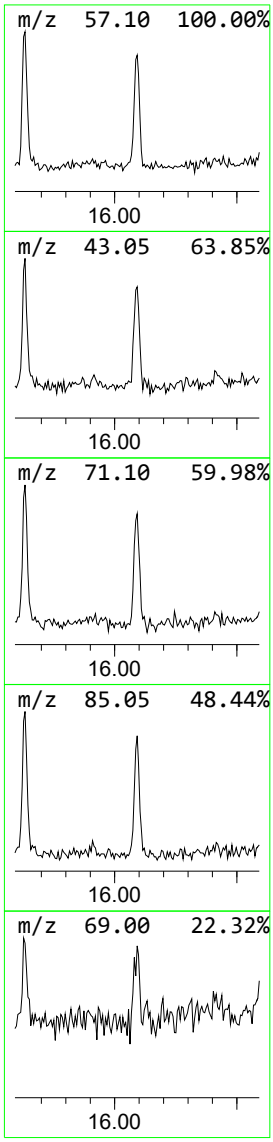
****

Peak Number 5 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.092	2.16 ng	55824	Perylene-d12	15.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Heneicosane	296	C21H44	000629-94-7	83
4	Pentacosane	352	C25H52	000629-99-2	80
5	Octacosane	394	C28H58	000630-02-4	80





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

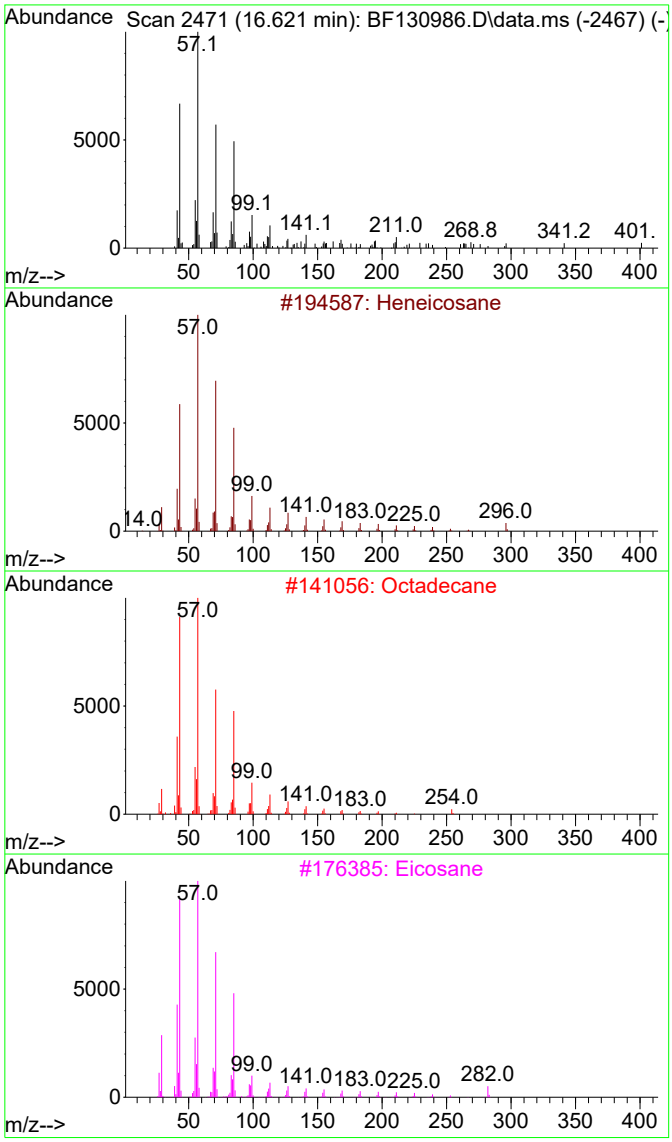
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

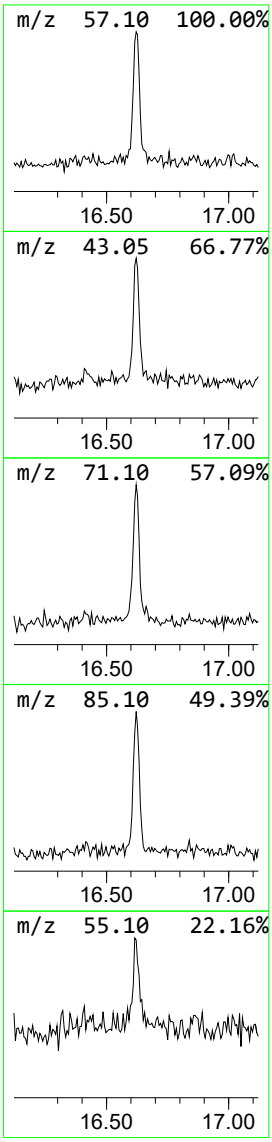
****

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.621	2.74 ng	70880	Perylene-d12	15.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Octadecane	254	C18H38	000593-45-3	87
3	Eicosane	282	C20H42	000112-95-8	87
4	Hexadecane	226	C16H34	000544-76-3	86
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86





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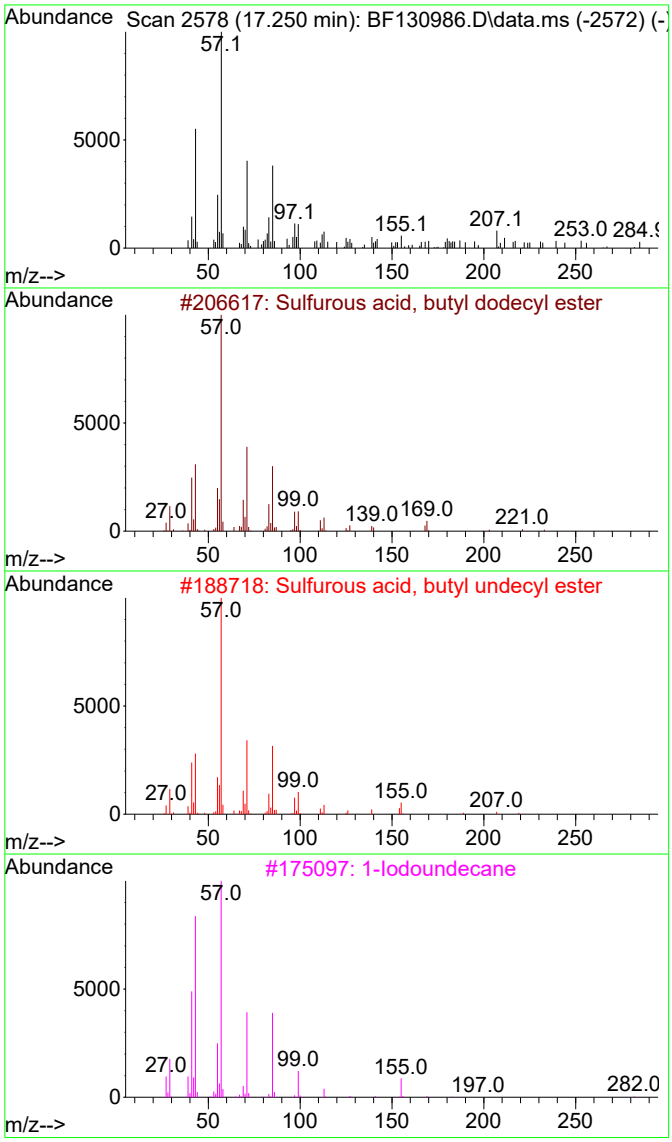
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

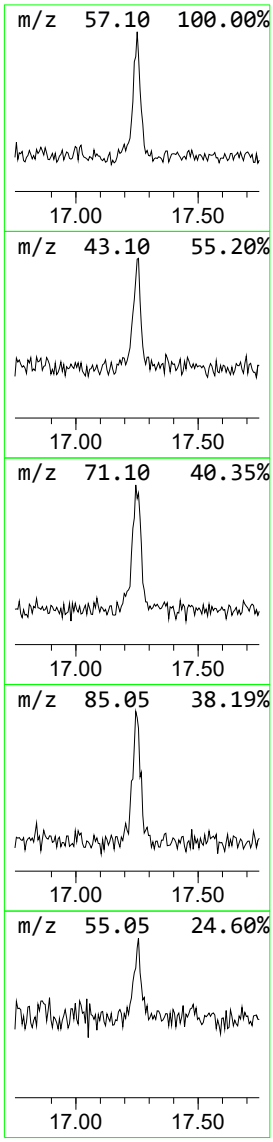
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Sulfurous acid, butyl dodec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.250	2.81 ng	72767	Perylene-d12	15.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
2	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	86
3	1-Iodoundecane	282	C11H23I	004282-44-4	74
4	Decane	142	C10H22	000124-18-5	72
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	68





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.275	4.8	ng	148271	1	6.910	622856	20.0
Propane, 1,1-di...	2.387	2.0	ng	63544	1	6.910	622856	20.0
2-Pentanone, 4-...	5.157	13.5	ng	420630	1	6.910	622856	20.0
Triphenylphosph...	14.198	2.9	ng	92844	5	14.104	631948	20.0
Tetracosane	16.092	2.2	ng	55824	6	15.615	517308	20.0
Heneicosane	16.621	2.7	ng	70880	6	15.615	517308	20.0
Sulfurous acid,...	17.250	2.8	ng	72767	6	15.615	517308	20.0