LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131029.D
Acq On : 05 Nov 2022 20:25
Operator : CG\JU
Sample : N5378-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5-A

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: BF131029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	11	18	27	rVB	493543	620523	33.13%	4.694%
2	2.299	32	36	46	rVB	34775	48606	2.60%	0.368%
3	5.128	512	517	526	rVB	217202	248400	13.26%	1.879%
4	5.522	579	584	587	rBV	1663192	1528062	81.58%	11.559%
5	6.528	749	755	758	rBV	1616599	1627793	86.91%	12.314%
6	6.904	815	819	822	rVB	465918	407274	21.74%	3.081%
7	7.463	909	914	917	rBV	1121064	1104760	58.98%	8.357%
8	8.092	1017	1021	1030	rBV2	27280	57068	3.05%	0.432%
9	8.186	1033	1037	1040	rBV	786497	646318	34.51%	4.889%
10	9.263	1215	1220	1223	rBV	2307194	1872972	100.00%	14.169%
11	9.375	1235	1239	1250	rVB	49955	54790	2.93%	0.414%
12	9.945	1332	1336	1340	rBV	866258	699457	37.34%	5.291%
13	10.739	1466	1471	1474	rBV	1391308	1153108	61.57%	8.723%
14	11.439	1586	1590	1593	rBV	724170	596960	31.87%	4.516%
15	11.504	1598	1601	1605	rVB2	27836	27285	1.46%	0.206%
16	12.533	1771	1776	1780	rVB	79329	68616	3.66%	0.519%
17	12.886	1831	1836	1839	rBV	29565	33908	1.81%	0.257%
18	13.027	1856	1860	1863	rBV	1511603	1282947	68.50%	9.705%
19	14.004	2018	2026	2032	rBV7	16893	53087	2.83%	0.402%
20	14.086	2032	2040	2043	rBV	425473	403550	21.55%	3.053%
21	14.180	2051	2056	2060	rBV	68355	71109	3.80%	0.538%
22	15.139	2213	2219	2222	rBV	31325	45871	2.45%	0.347%
23	15.515	2278	2283	2290	rBV	28091	41514	2.22%	0.314%
24	15.586	2290	2295	2303	rBV	320212	409949	21.89%	3.101%
25	16.056	2371	2375	2380	rVB2	17739	26569	1.42%	0.201%
26	16.586	2459	2465	2472	rBV3	16889	33952	1.81%	0.257%
27	17.209	2564	2571	2577	rBV5	13969	30658	1.64%	0.232%
28	17.939	2690	2695	2700	rBV5	12195	24147	1.29%	0.183%

Sum of corrected areas: 13219253

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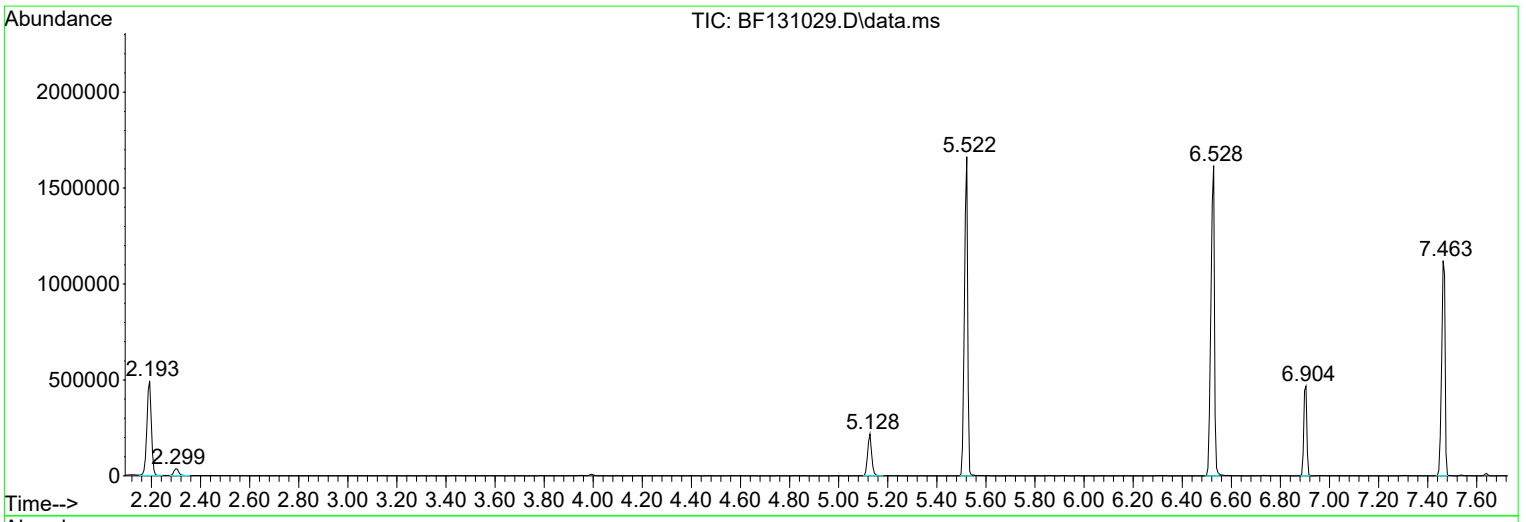
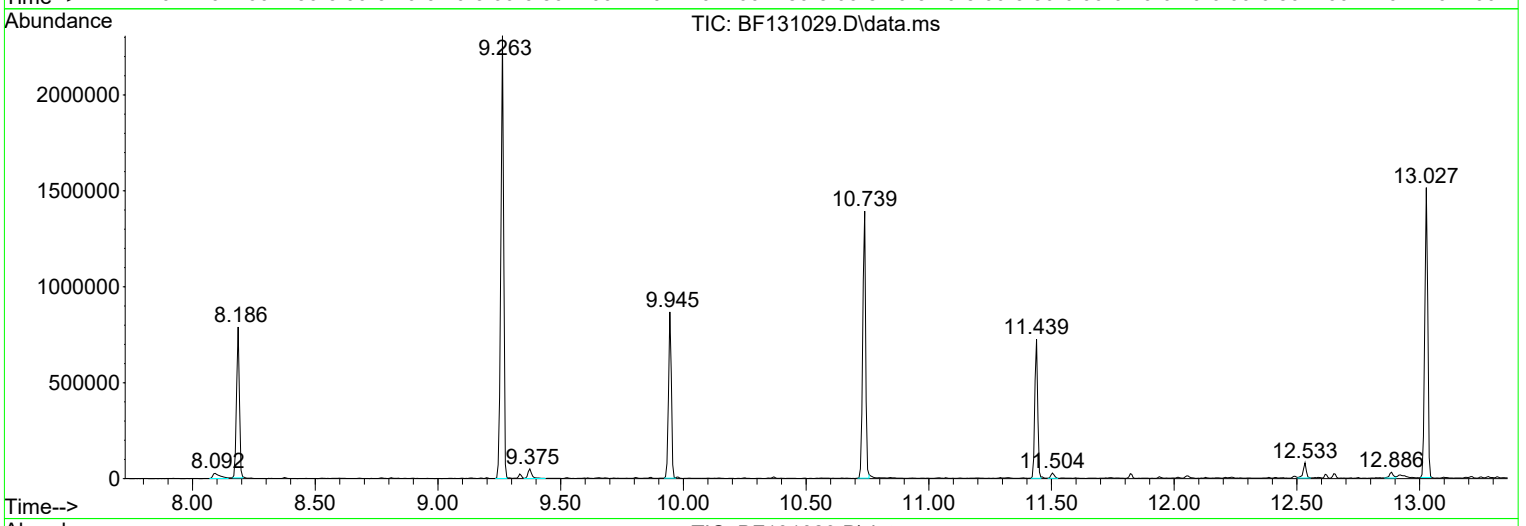
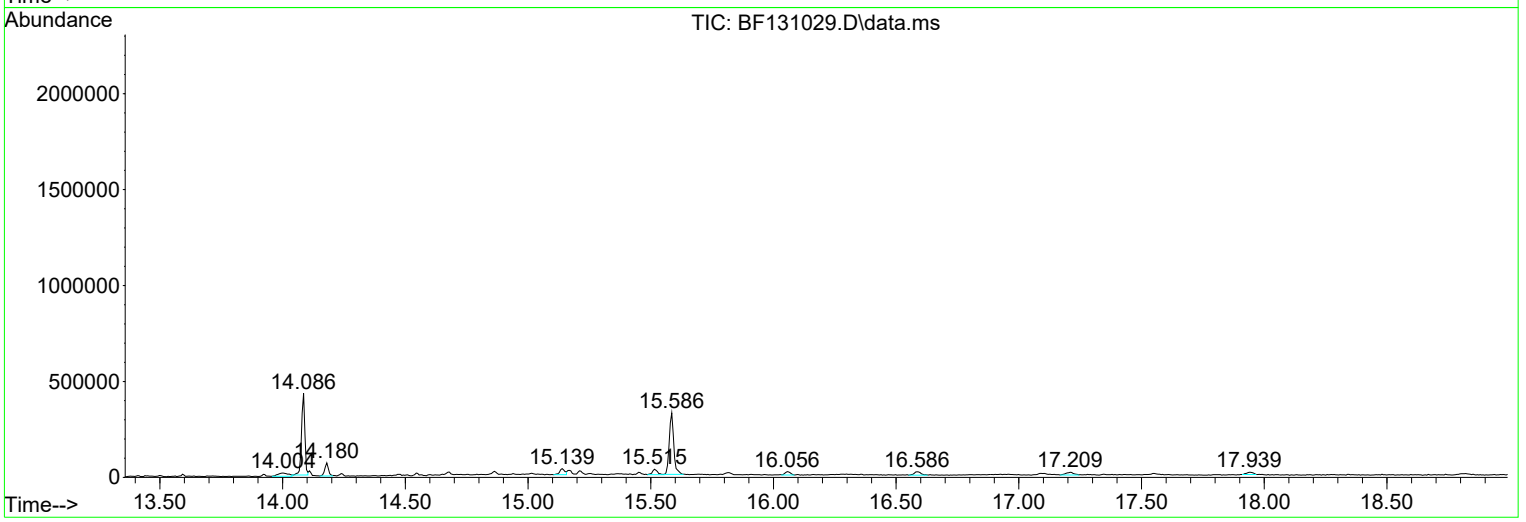
Instrument :
BNA_F
ClientSampleId :
SB-16-20221028-10.5-11.5-A

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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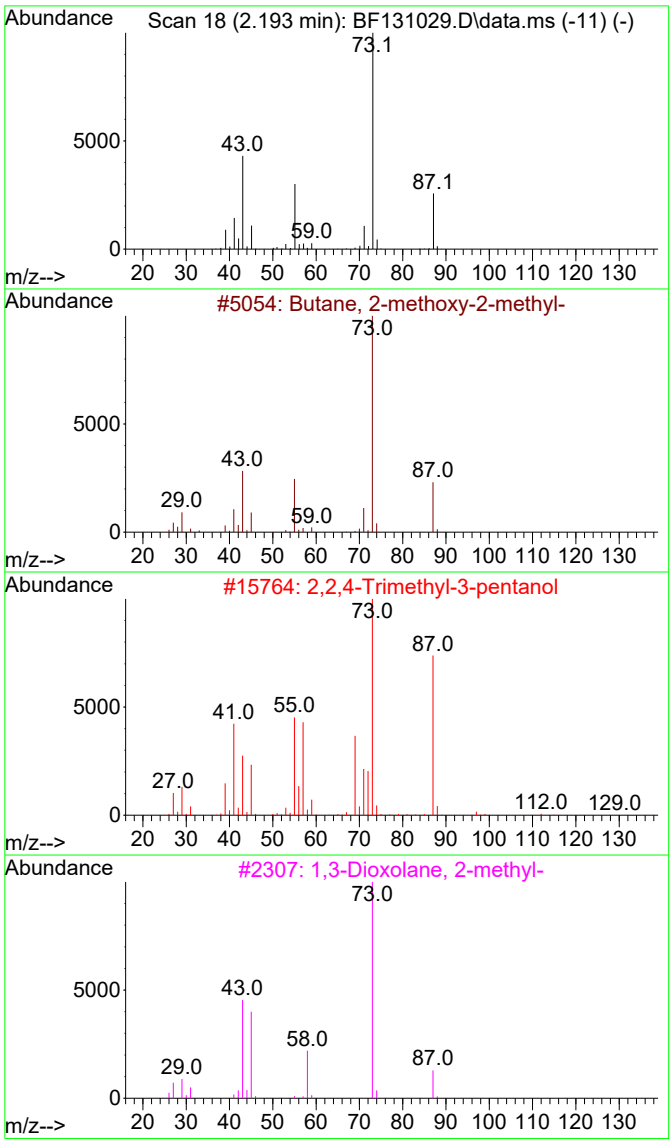
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

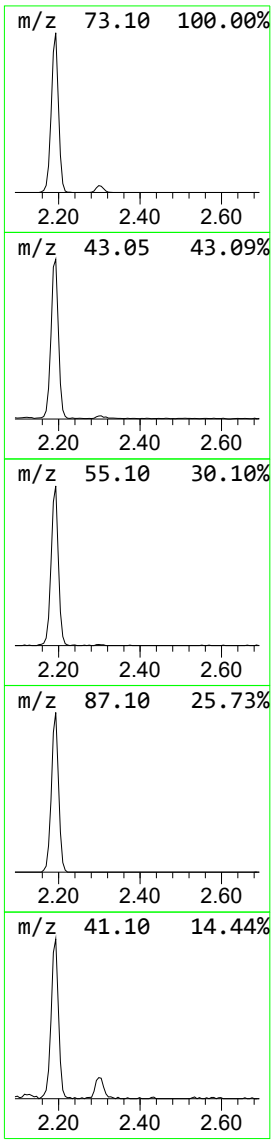
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	30.47 ng	620523	1,4-Dichlorobenzene-d4	6.904

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Sample : N5378-05
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Instrument :
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ClientSampleId :
SB-16-20221028-10.5-11.5-A

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

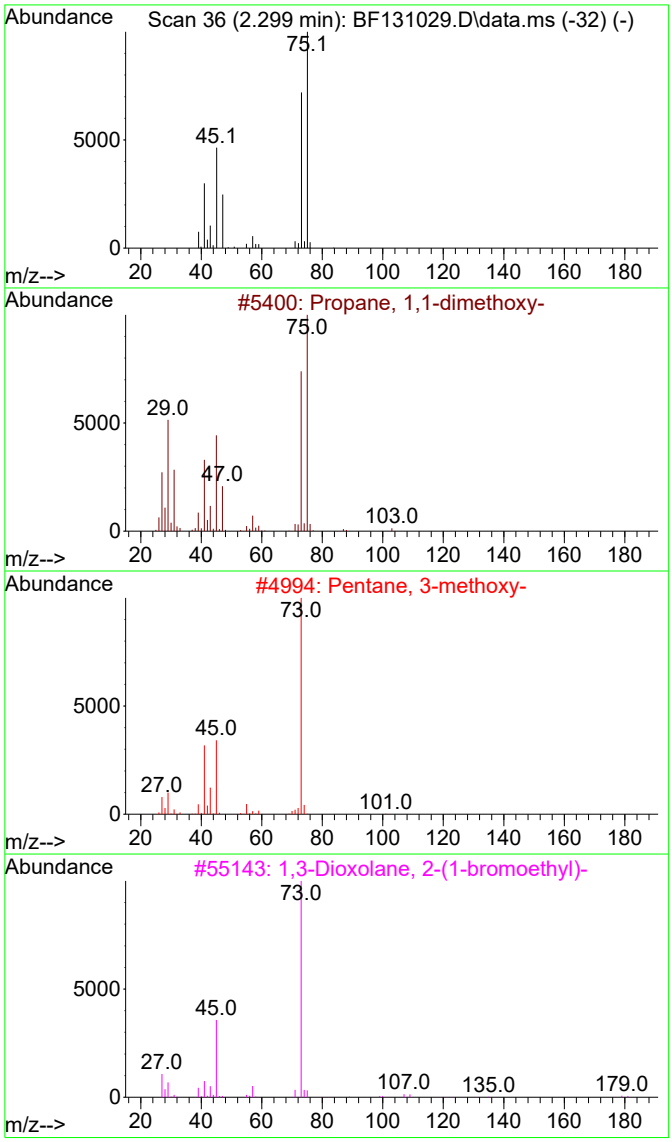
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

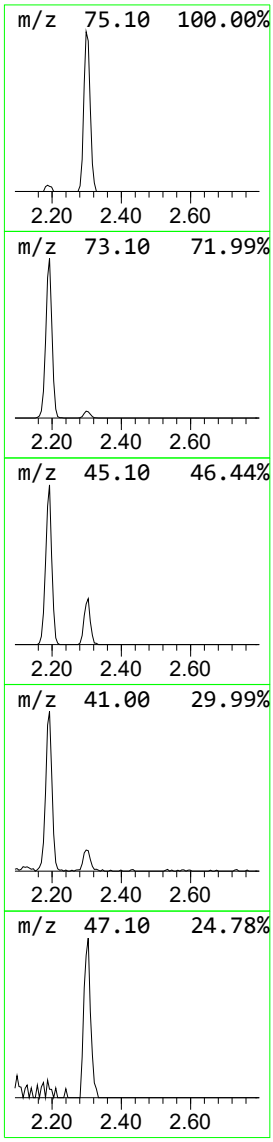
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	2.39 ng	48606	1,4-Dichlorobenzene-d4	6.904

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	12
3	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	7
5	Glycine	75	C2H5NO2	000056-40-6	4





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SB-16-20221028-10.5-11.5-A

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

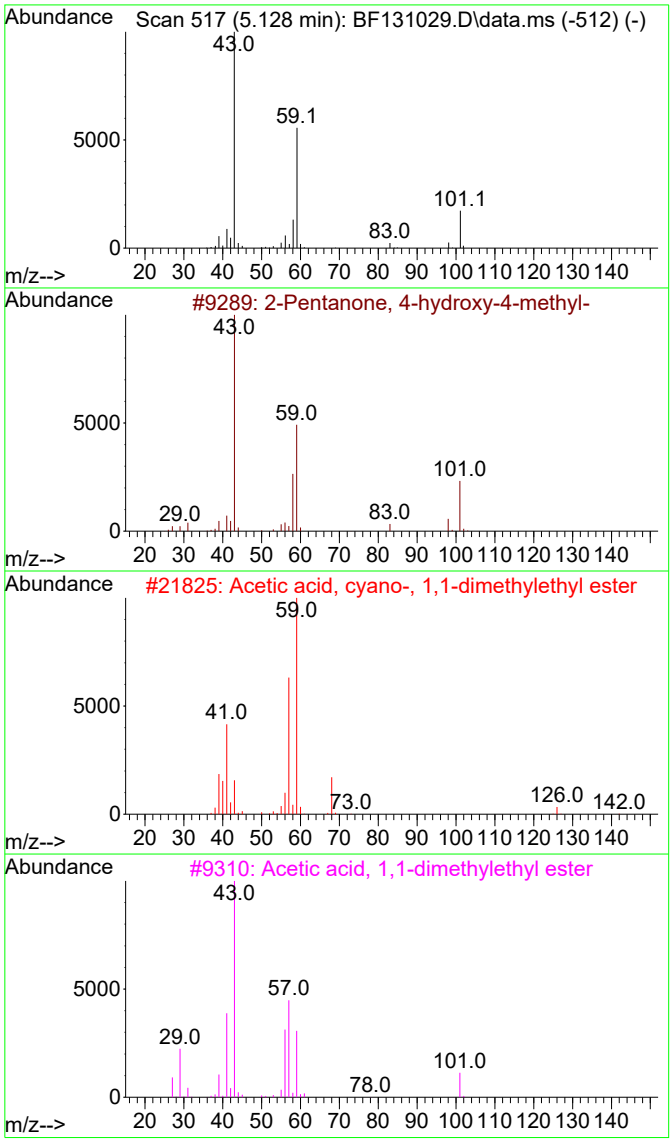
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

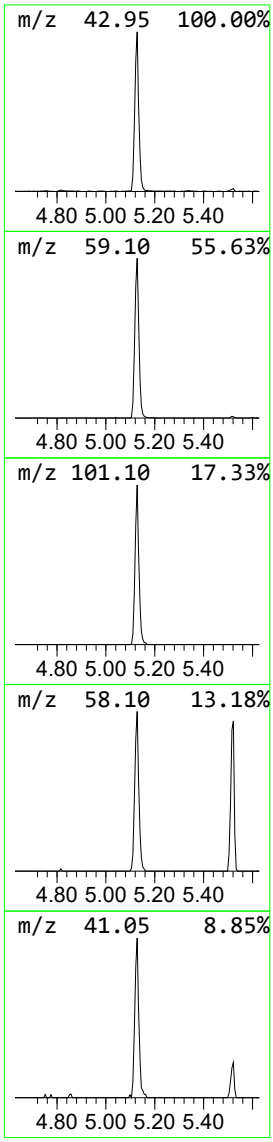
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	12.20 ng	248400	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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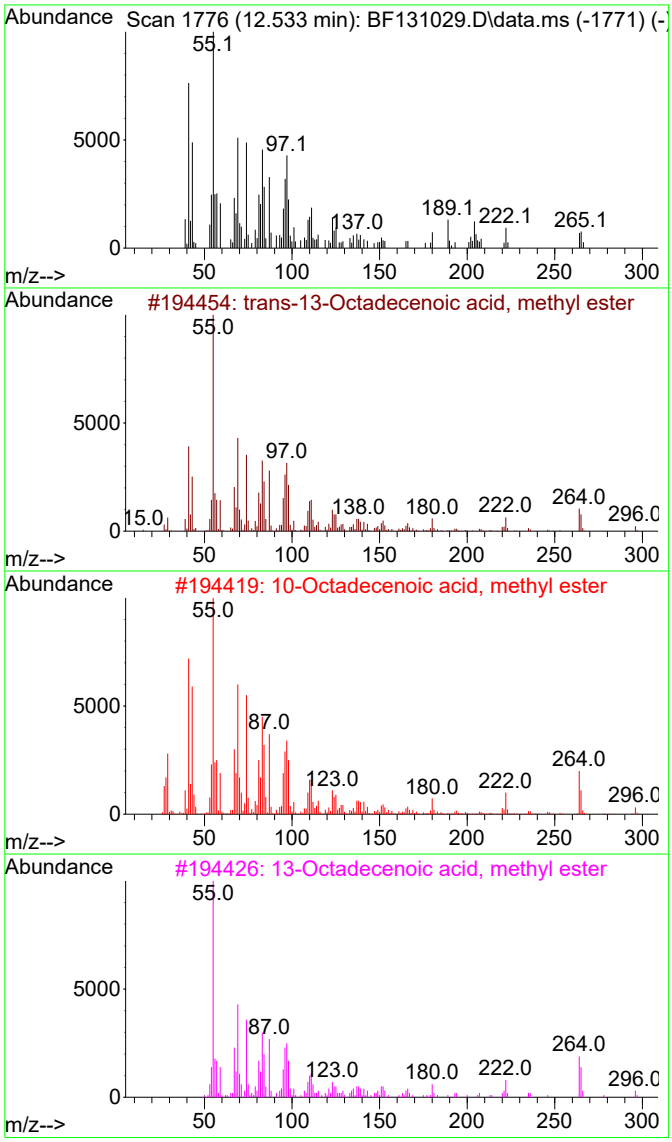
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

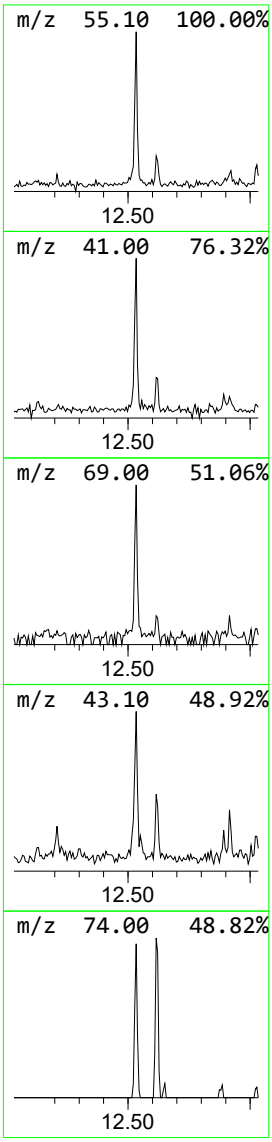
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 trans-13-Octadecenoic acid,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	2.30 ng	68616	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	83





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

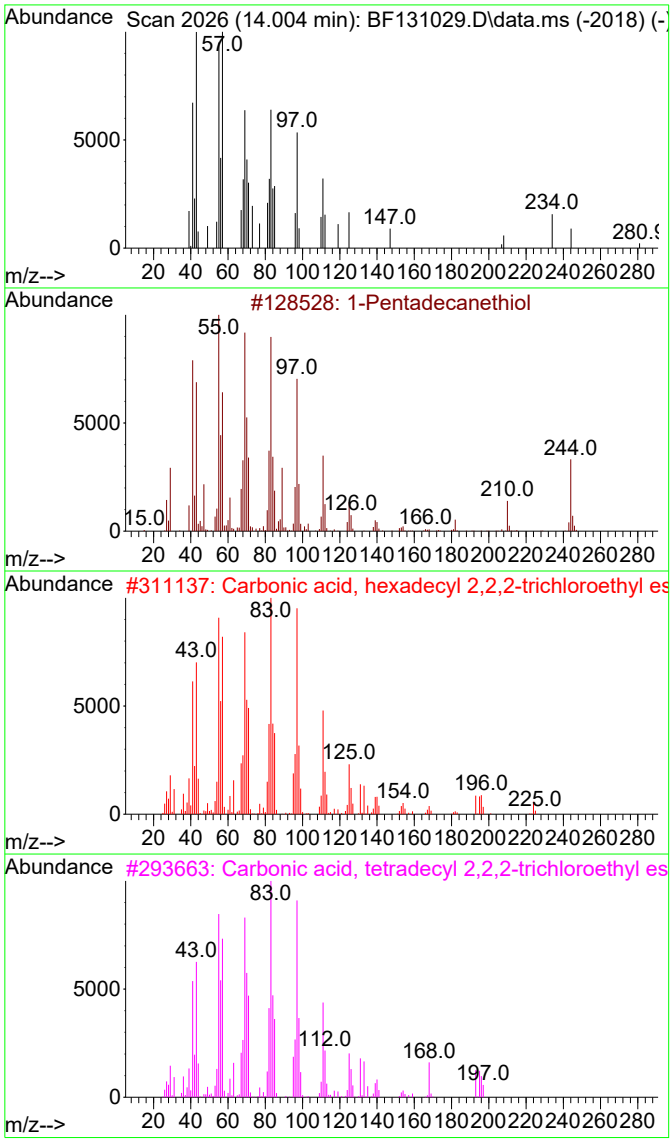
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

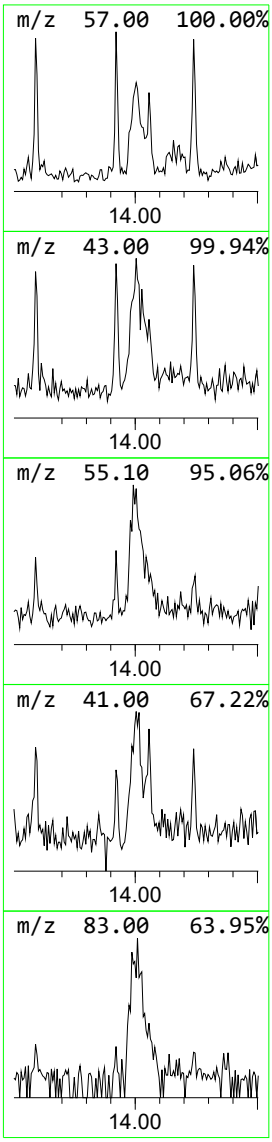
****

Peak Number 5 1-Pentadecanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	2.63 ng	53087	Chrysene-d12	14.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol	244	C15H32S	025276-70-4	91
2	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	87
3	Carbonic acid, tetradecyl 2,2,2-...	388	C17H31Cl3O3	1000314-56-0	87
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	83
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83





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

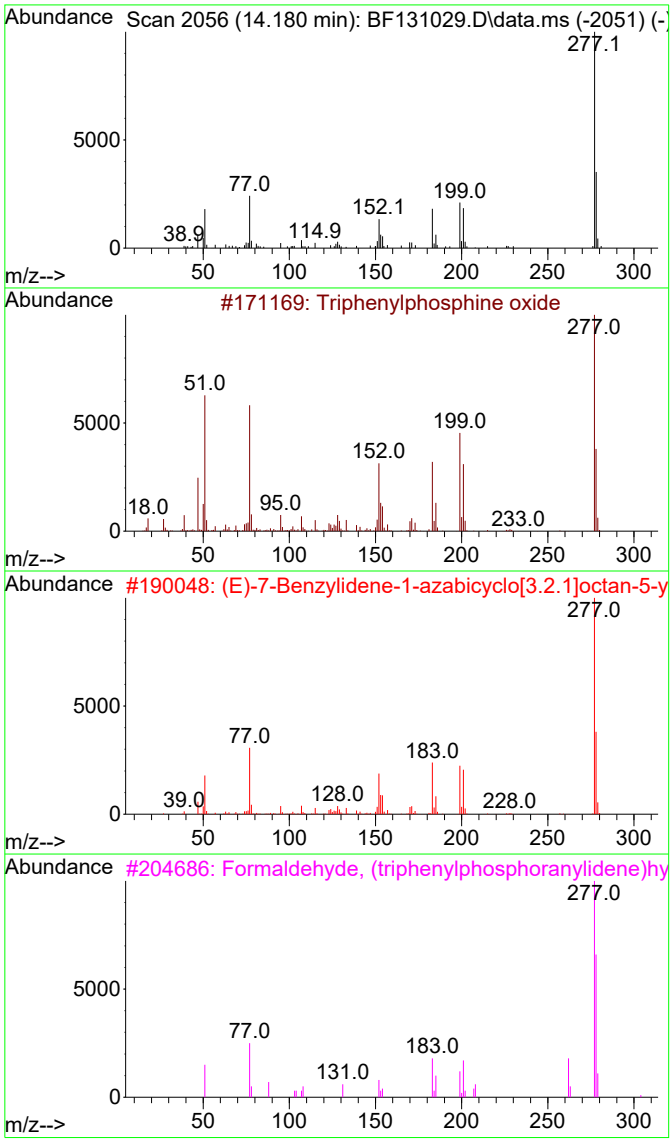
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

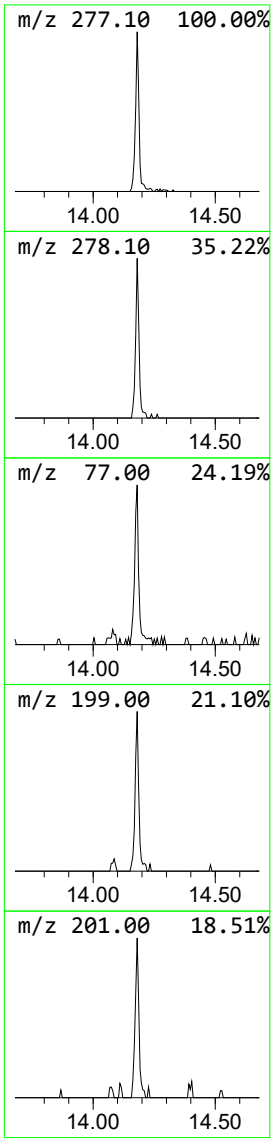
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.180	3.52 ng	71109	Chrysene-d12	14.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	70
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	28
5	1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	23





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...	2.193	30.5	ng	620523	1	6.904	407274	20.0
Propane, 1,1-di...	2.299	2.4	ng	48606	1	6.904	407274	20.0
2-Pentanone, 4-...	5.128	12.2	ng	248400	1	6.904	407274	20.0
trans-13-Octade...	12.533	2.3	ng	68616	4	11.439	596960	20.0
1-Pentadecanethiol	14.004	2.6	ng	53087	5	14.086	403550	20.0
Triphenylphosph...	14.180	3.5	ng	71109	5	14.086	403550	20.0