LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122221\
Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126325.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.410	390	395	402	rBV	467710	537885	12.19%	1.731%
2	5.040	495	502	511	rBV	1428099	2108584	47.80%	6.786%
3	5.440	564	570	573	rBV	3992285	4291879	97.29%	13.813%
4	5.834	633	637	649	rVB	229575	200766	4.55%	0.646%
5	6.445	735	741	744	rBV	3637261	4236790	96.04%	13.635%
6	6.816	800	804	807	rBV	1146348	896682	20.33%	2.886%
7	7.381	894	900	903	rBV	2759009	2894078	65.60%	9.314%
8	8.098	1017	1022	1038	rBV	1331238	1247520	28.28%	4.015%
9	9.175	1200	1205	1229	rBV	3784329	4411422	100.00%	14.197%
10	9.851	1316	1320	1335	rBV	1210756	1266204	28.70%	4.075%
11	10.639	1450	1454	1479	rBV	2259190	2447057	55.47%	7.875%
12	11.333	1569	1572	1590	rBV	1051889	1163797	26.38%	3.745%
13	12.927	1838	1843	1846	rBV	3194886	3220555	73.00%	10.365%
14	13.974	2017	2021	2033	rBV	597703	692607	15.70%	2.229%
15	14.068	2033	2037	2048	rVB	115013	146416	3.32%	0.471%
16	15.092	2206	2211	2220	rBV	55095	63333	1.44%	0.204%
17	15.421	2262	2267	2272	rBV2	428957	644565	14.61%	2.074%
18	15.468	2272	2275	2285	rVB	97839	143961	3.26%	0.463%
19	15.898	2342	2348	2358	rBV	74601	119275	2.70%	0.384%
20	16.398	2426	2433	2440	rBV2	70055	128826	2.92%	0.415%
21	16.980	2526	2532	2540	rVB2	49638	107111	2.43%	0.345%
22	17.668	2641	2649	2661	rBV3	39519	102849	2.33%	0.331%

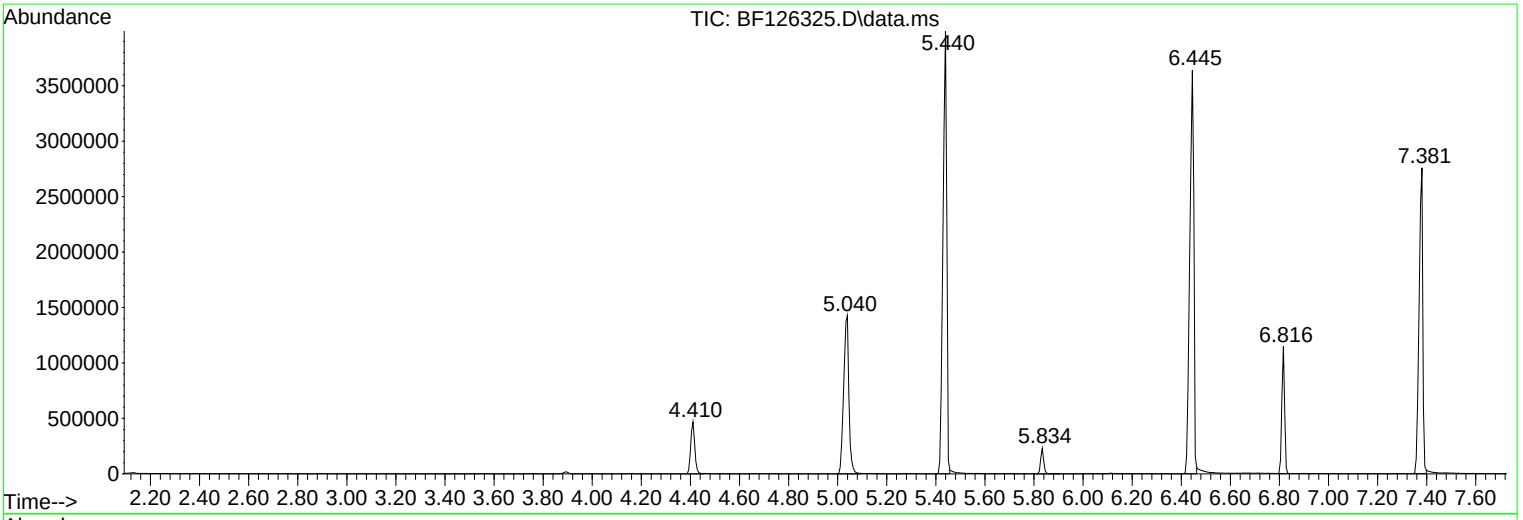
Sum of corrected areas: 31072162

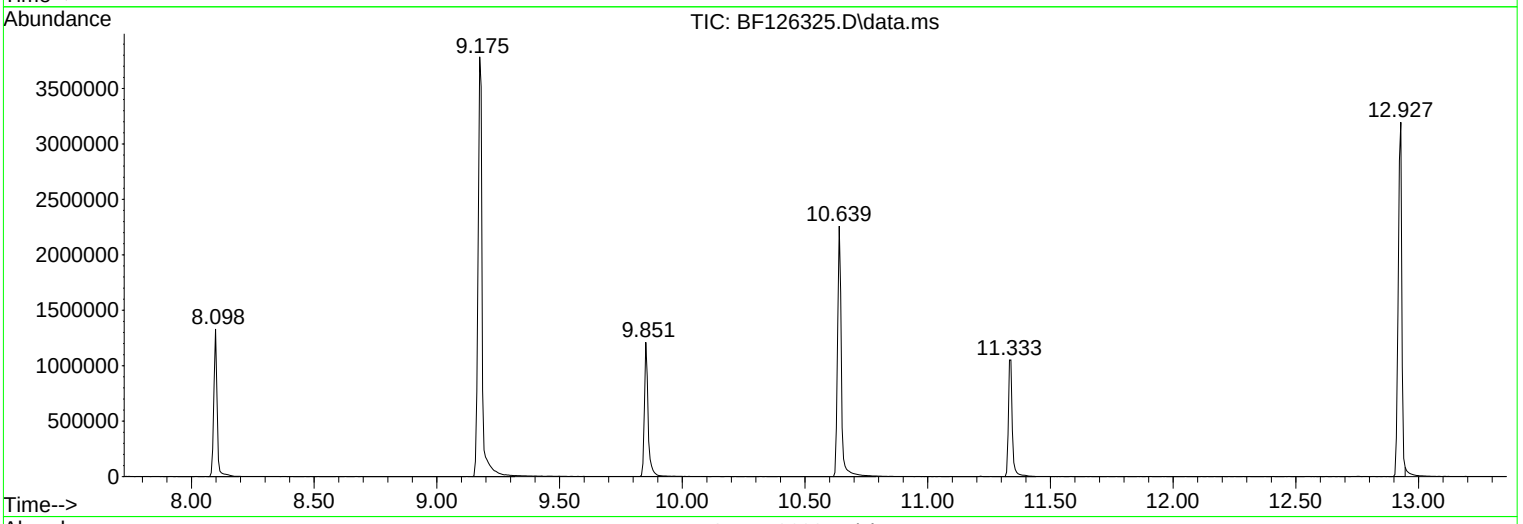
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122221\
Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

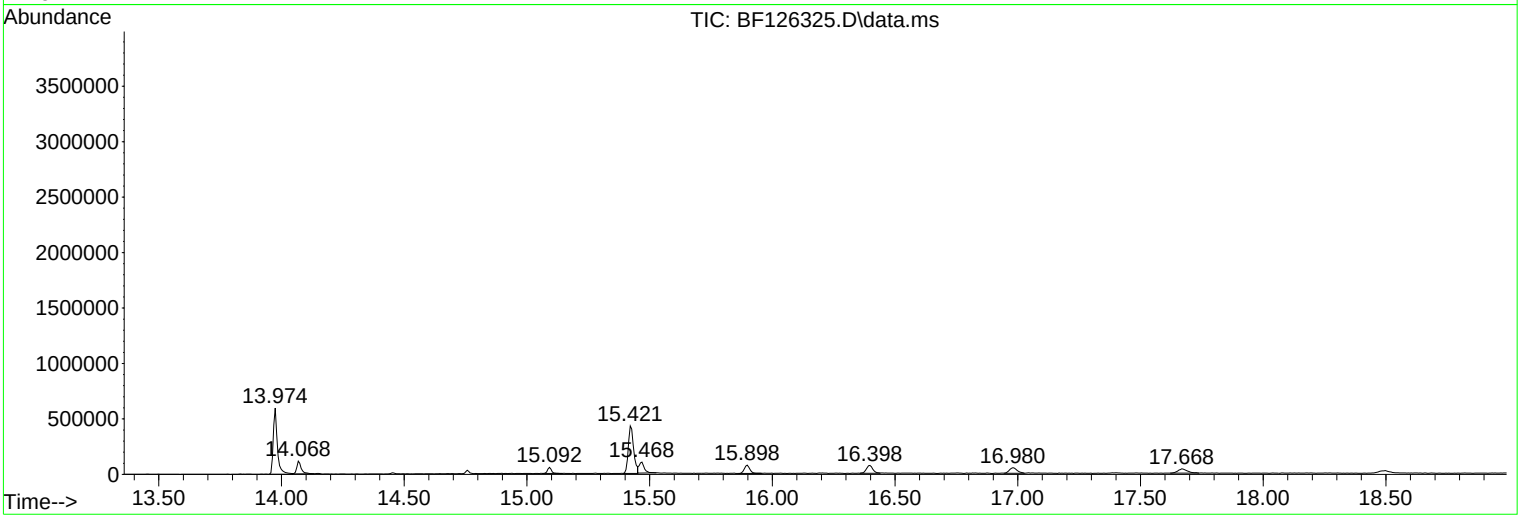
Instrument :
BNA_F
ClientSampleId :
PB141549BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122221\
Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

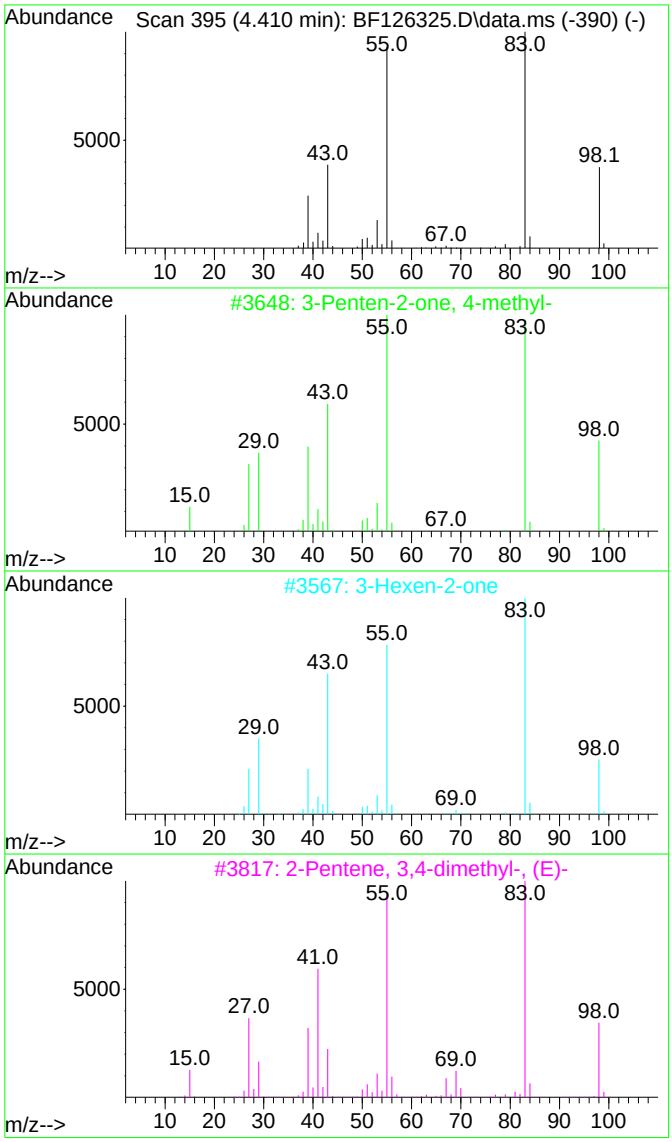
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

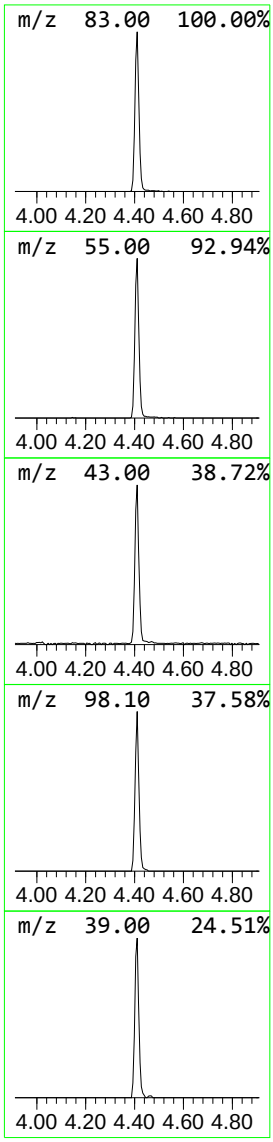
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.410	12.00 ng	537885	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122221\
Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

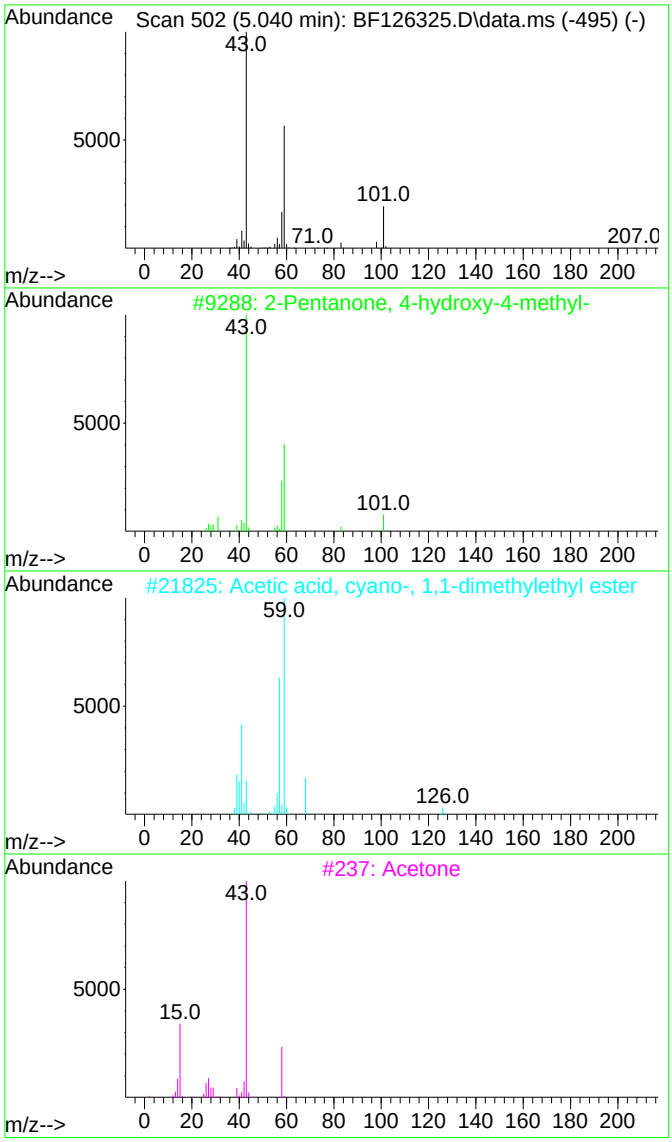
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

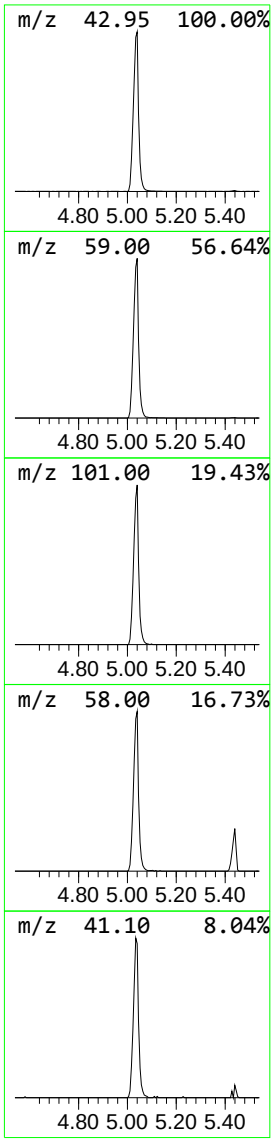
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	47.03 ng	2108580	1,4-Dichlorobenzene-d4	6.816

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	17
3	Acetone	58	C3H6O	000067-64-1	9
4	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

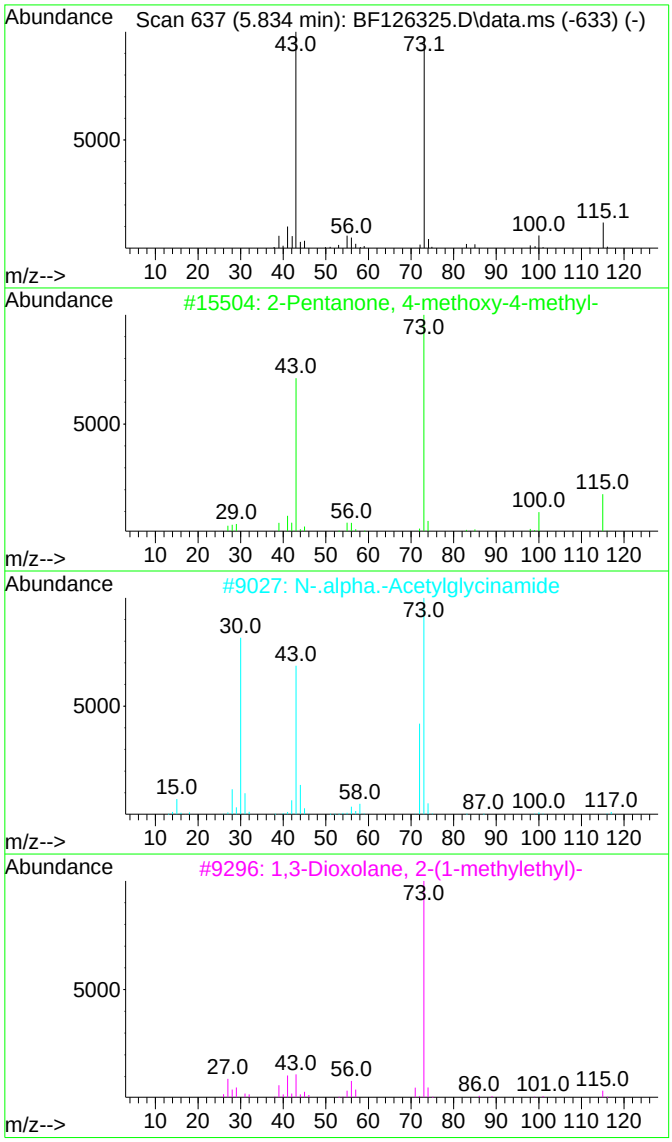
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

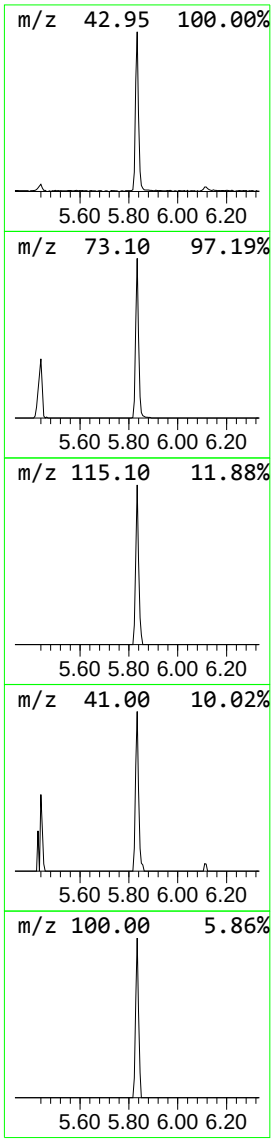
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	4.48 ng	200766	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122221\
Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

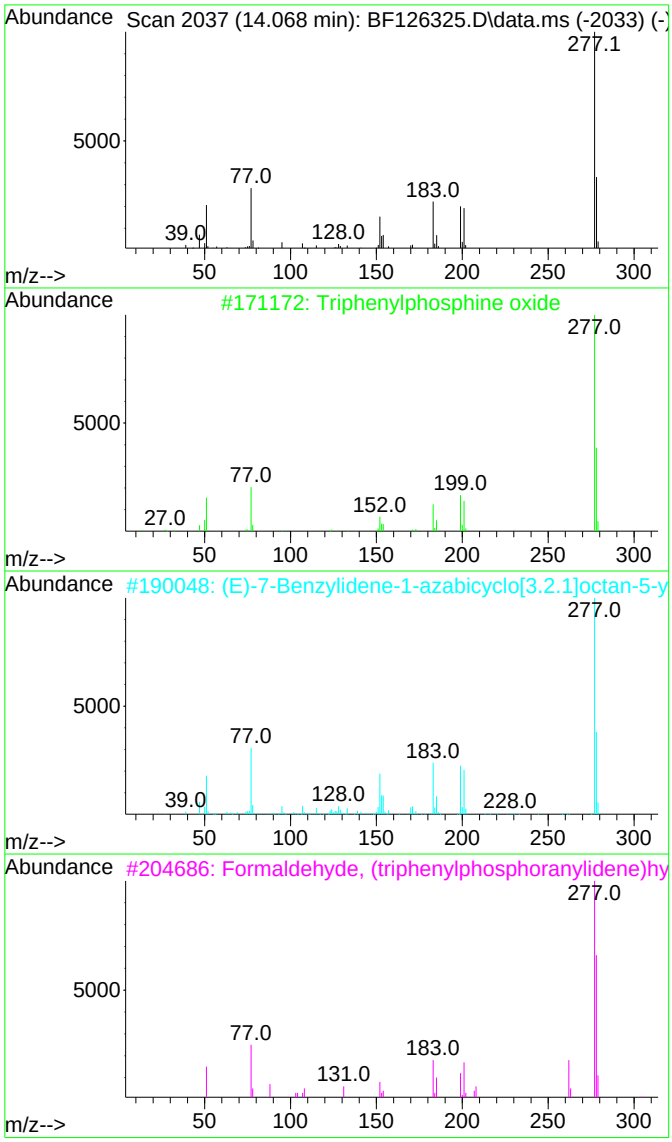
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

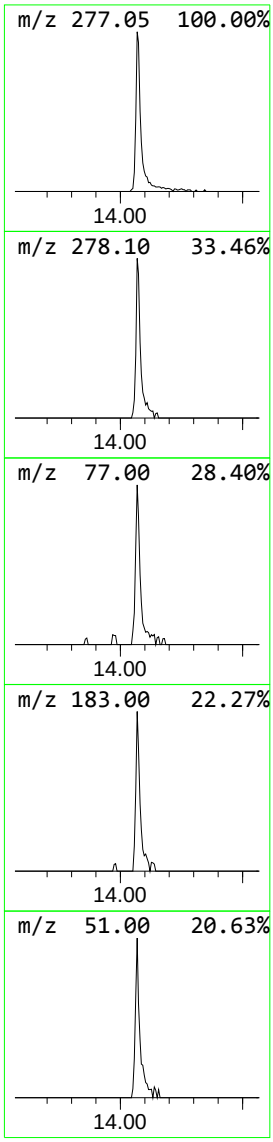
****

Peak Number 4 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.069	4.23 ng	146416	Chrysene-d12	13.974

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	64
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122221\
Data File : BF126325.D
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Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

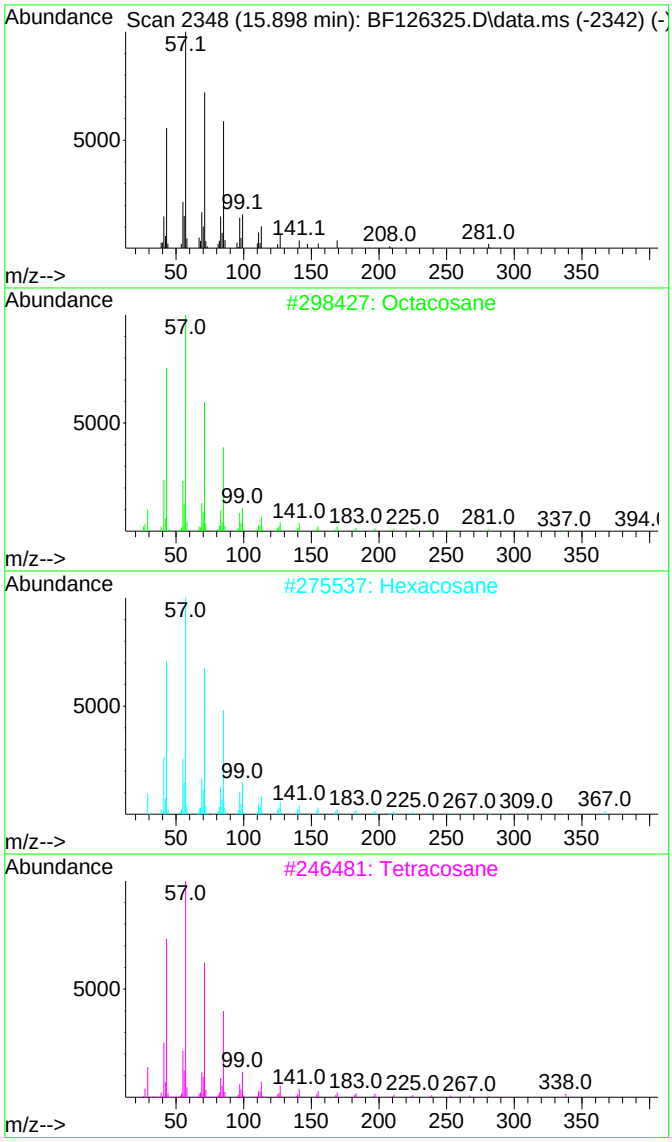
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

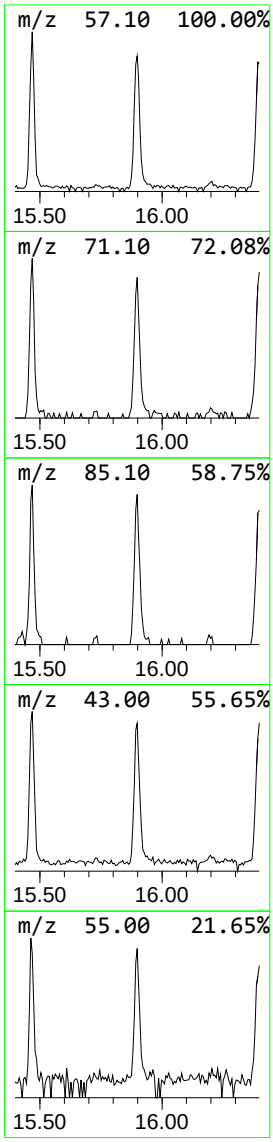
****

Peak Number 5 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	3.70 ng	119275	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Tetracosane	338	C24H50	000646-31-1	86
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122221\
Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

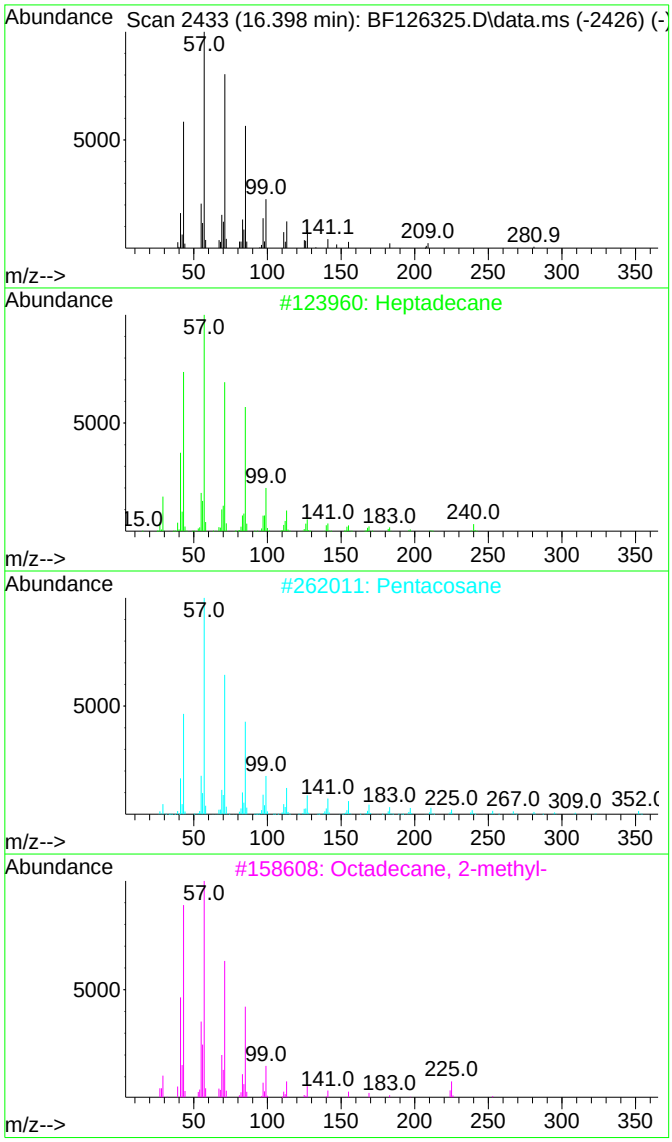
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

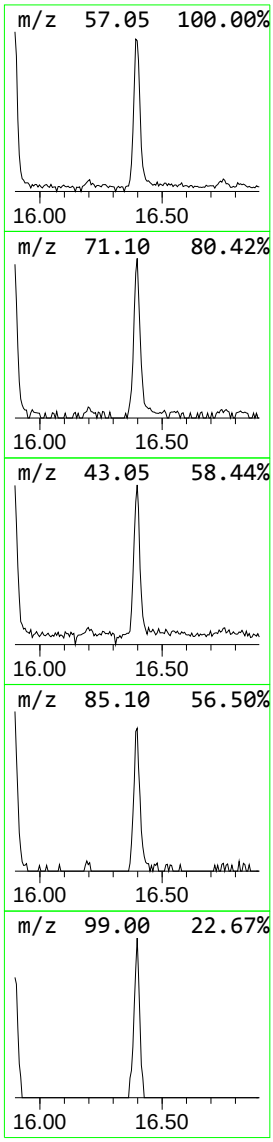
****

Peak Number 6 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.398	4.00 ng	128826	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Pentacosane	352	C25H52	000629-99-2	86
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
4	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	64
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	52





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Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

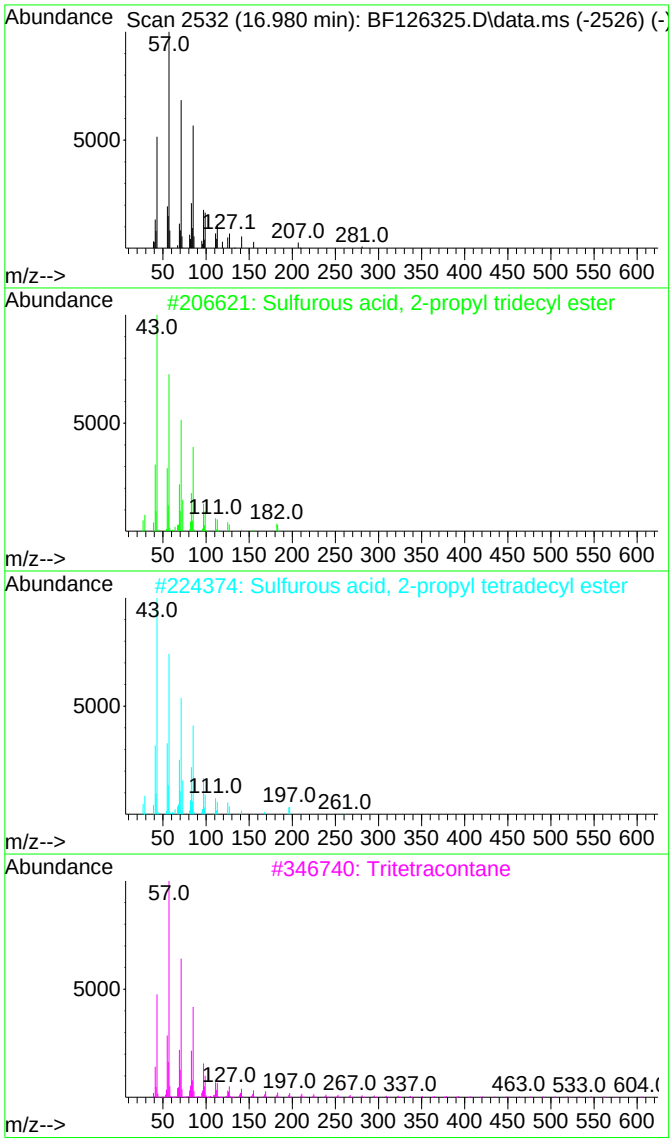
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

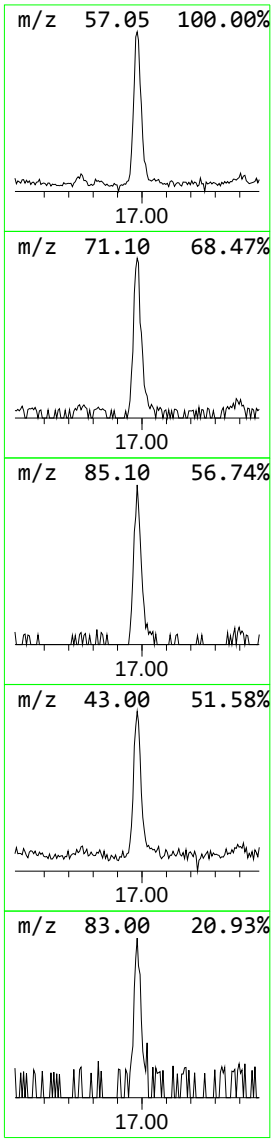
****

Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.980	3.32 ng	107111	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	90
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1010309-12-5	90
3	Tritetracontane	605	C43H88	007098-21-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90





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Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

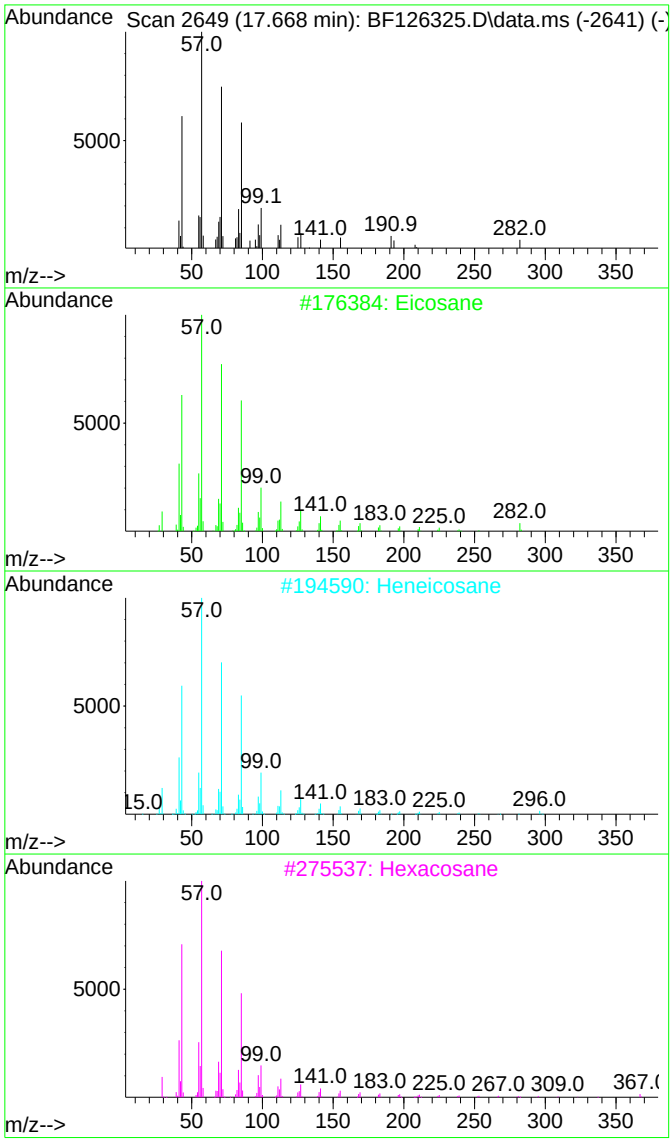
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

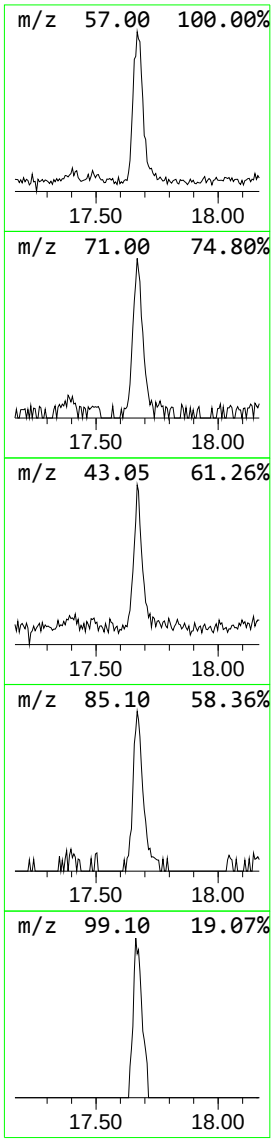
****

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.668	3.19 ng	102849	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Heptadecane	240	C17H36	000629-78-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122221\
Data File : BF126325.D
Acq On : 22 Dec 2021 12:52
Operator : JU/CG
Sample : PB141549BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141549BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.410	12.0	ng	537885	1	6.816	896682	20.0
2-Pentanone, 4-...	5.040	47.0	ng	2108580	1	6.816	896682	20.0
2-Pentanone, 4-...	5.834	4.5	ng	200766	1	6.816	896682	20.0
Triphenylphosph...	14.069	4.2	ng	146416	5	13.974	692607	20.0
Octacosane	15.898	3.7	ng	119275	6	15.421	644565	20.0
Heptadecane	16.398	4.0	ng	128826	6	15.421	644565	20.0
Sulfurous acid,...	16.980	3.3	ng	107111	6	15.421	644565	20.0
Eicosane	17.668	3.2	ng	102849	6	15.421	644565	20.0