LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
Data File : BF126277.D
Acq On : 20 Dec 2021 14:33
Operator : JU/CG
Sample : M5082-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(55-62)

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: BF126277.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	12	rVB	686325	694476	16.94%	2.587%
2	2.216	18	22	29	rVB	90088	113981	2.78%	0.425%
3	5.028	495	500	511	rVB	859129	1145541	27.95%	4.267%
4	5.434	564	569	572	rBV	3935900	4098955	100.00%	15.269%
5	5.834	633	637	642	rVB	137066	116567	2.84%	0.434%
6	6.445	735	741	757	rBV	3664643	3977913	97.05%	14.818%
7	6.816	801	804	808	rBV	1039178	815576	19.90%	3.038%
8	7.375	894	899	903	rBV	2392010	2504625	61.10%	9.330%
9	8.098	1018	1022	1026	rBV	1128568	941675	22.97%	3.508%
10	9.175	1200	1205	1208	rBV	3402860	3207415	78.25%	11.948%
11	9.263	1217	1220	1226	rVB2	58139	53406	1.30%	0.199%
12	9.851	1316	1320	1333	rVB	1005562	862510	21.04%	3.213%
13	10.639	1450	1454	1465	rBV	1850843	1746514	42.61%	6.506%
14	11.333	1569	1572	1576	rBV	848435	776687	18.95%	2.893%
15	11.869	1660	1663	1667	rBV	65331	72146	1.76%	0.269%
16	12.922	1838	1842	1846	rBV	2945147	2960867	72.23%	11.029%
17	13.874	1999	2004	2015	rBV3	182842	518480	12.65%	1.931%
18	13.969	2017	2020	2025	rVB	856162	862341	21.04%	3.212%
19	14.069	2033	2037	2042	rBV	357275	377359	9.21%	1.406%
20	14.833	2164	2167	2170	rVB	110498	108478	2.65%	0.404%
21	15.421	2262	2267	2272	rBV	709463	889953	21.71%	3.315%

Sum of corrected areas: 26845465

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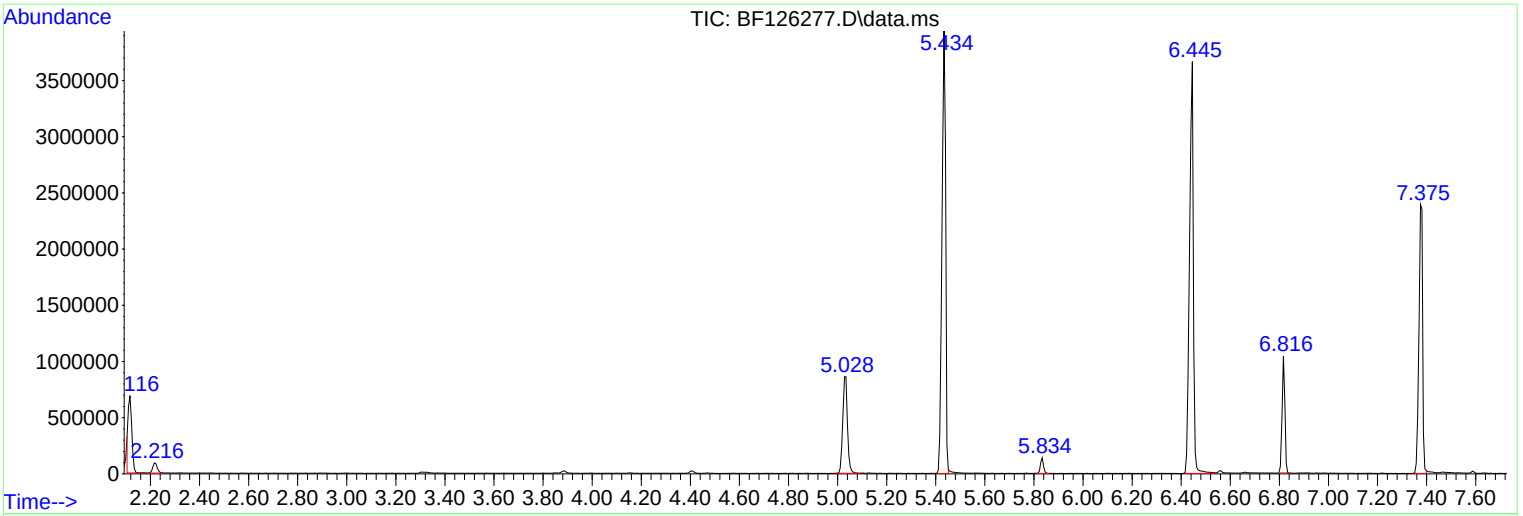
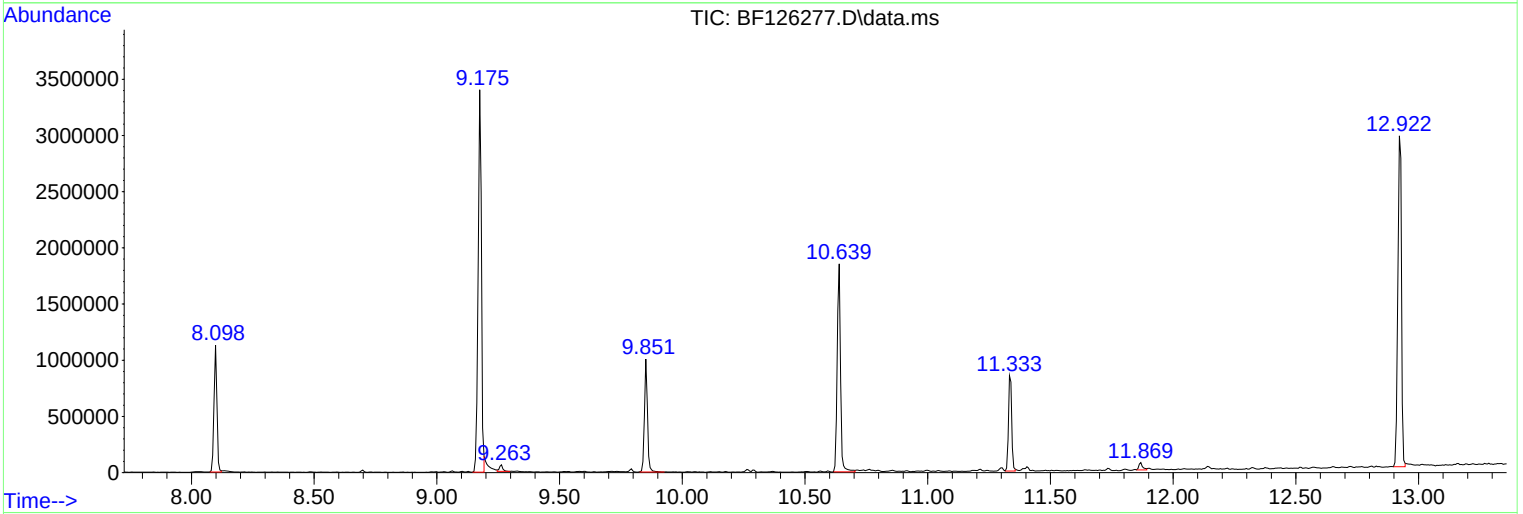
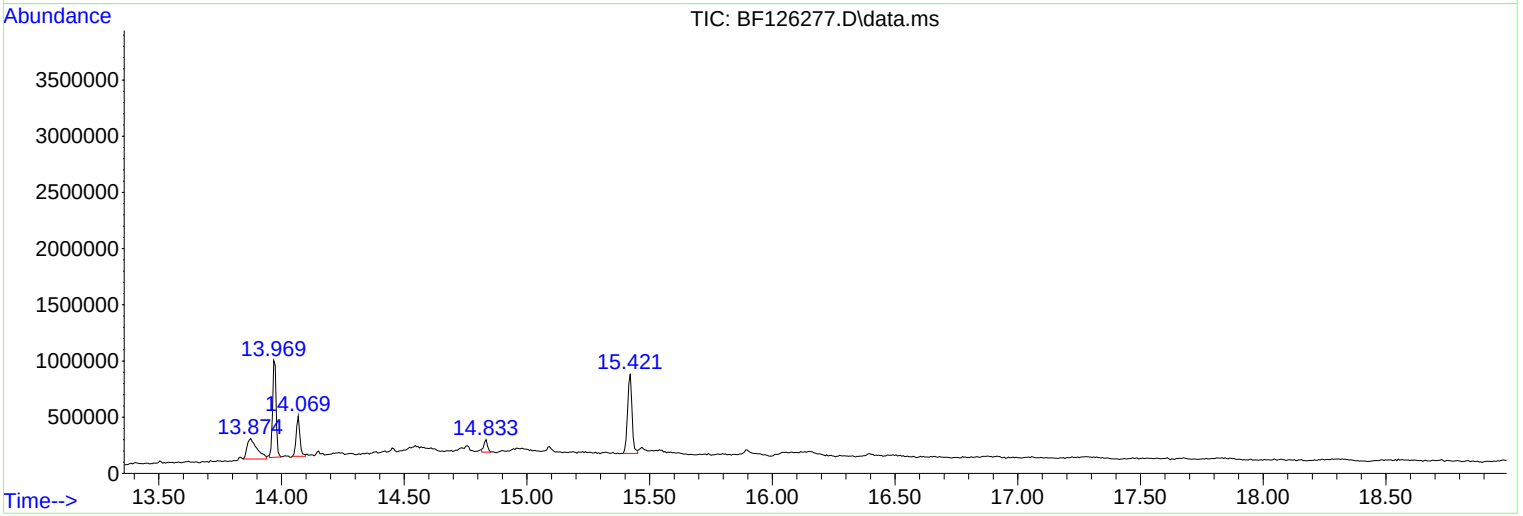
ClientSampleId :
SASP2-121-1(55-62)

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







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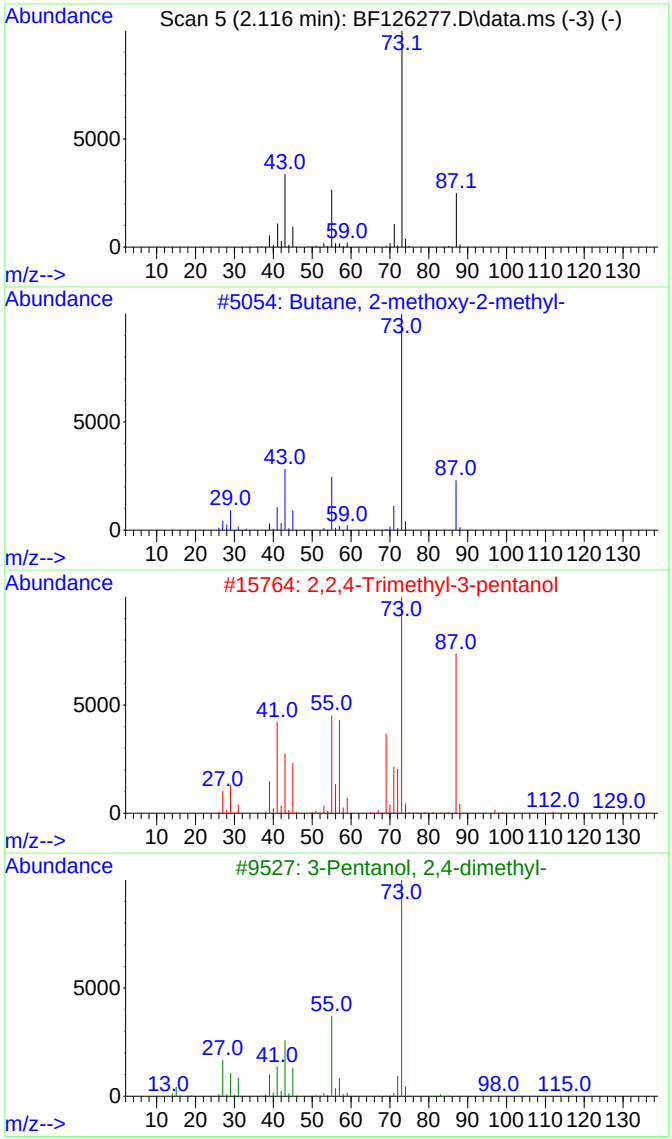
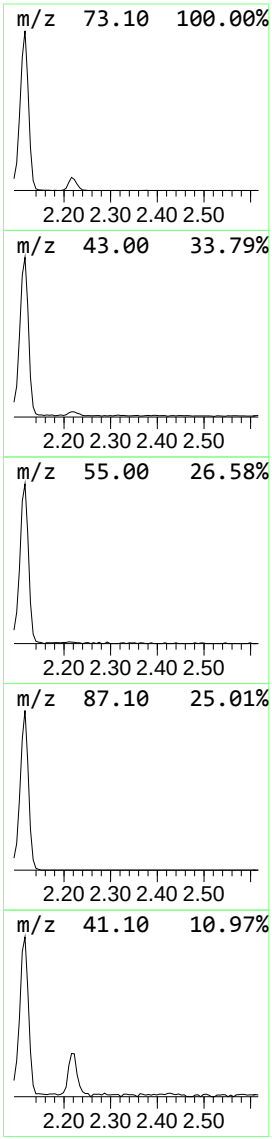
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	17.03 ng	694476	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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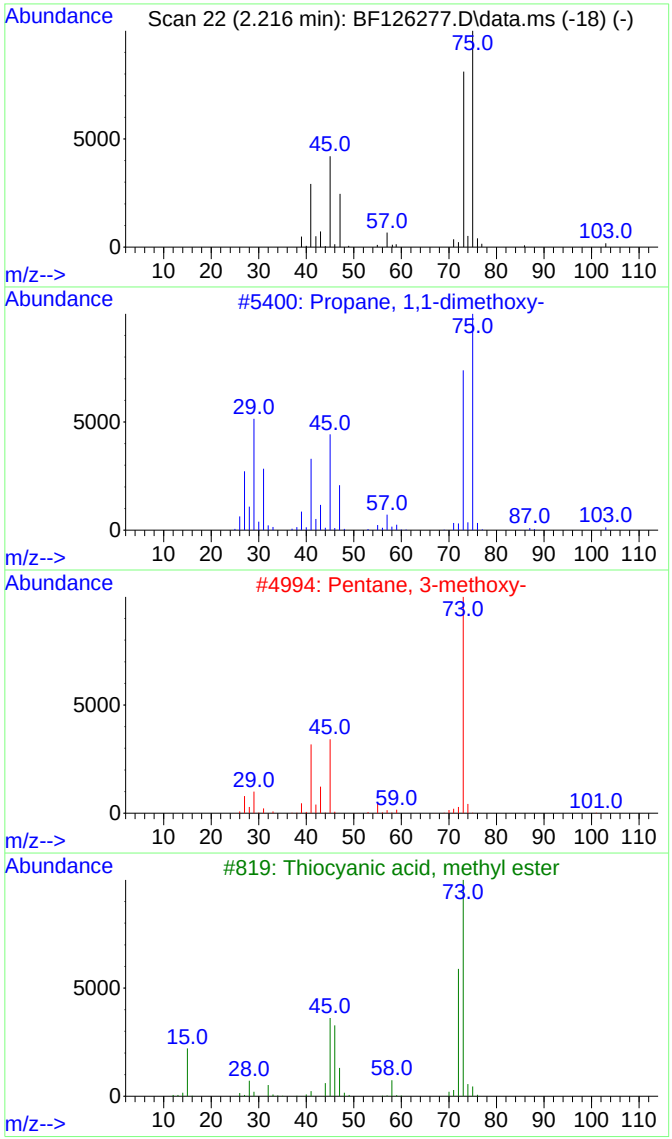
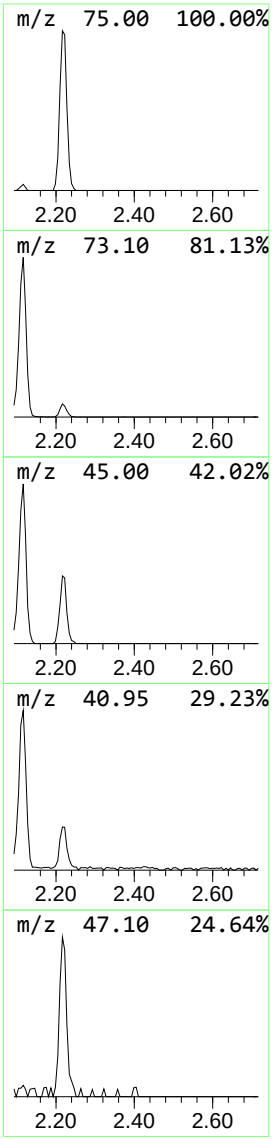
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	2.80 ng	113981	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	25
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	16
5	2-(3-Bromopropyl)-[1,3]dioxolane	194	C6H11BrO2	062563-07-9	12





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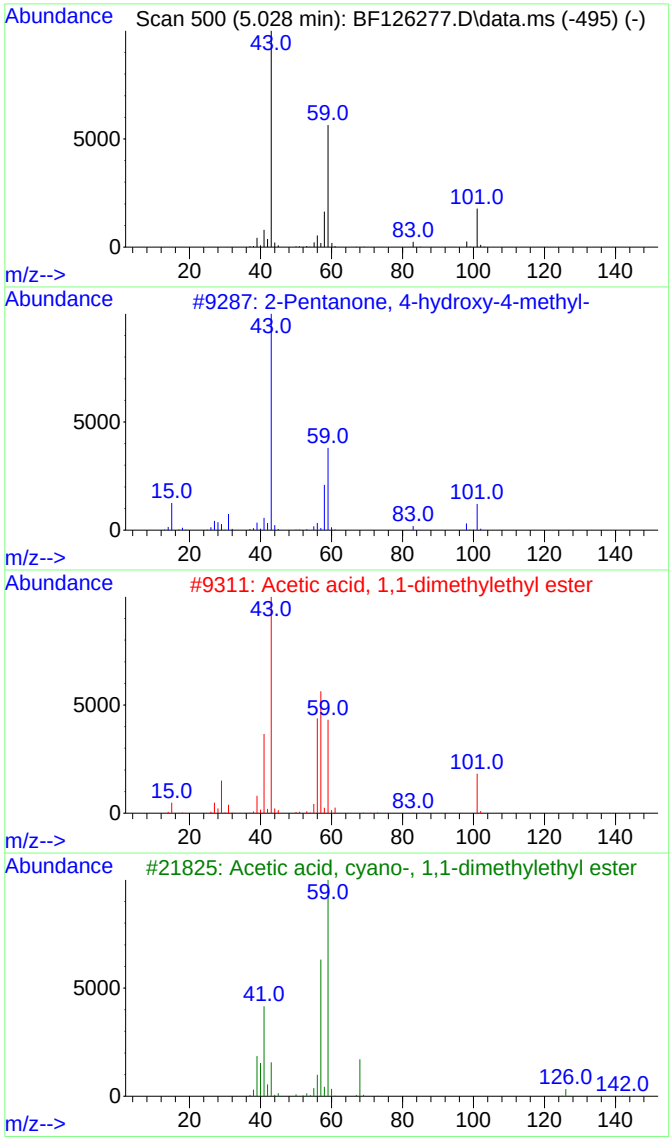
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

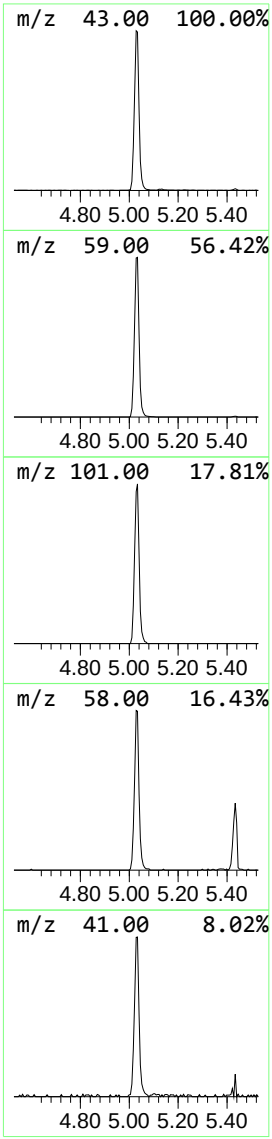
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	28.09 ng	1145540	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 20 Dec 2021 14:33
Operator : JU/CG
Sample : M5082-02
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Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(55-62)

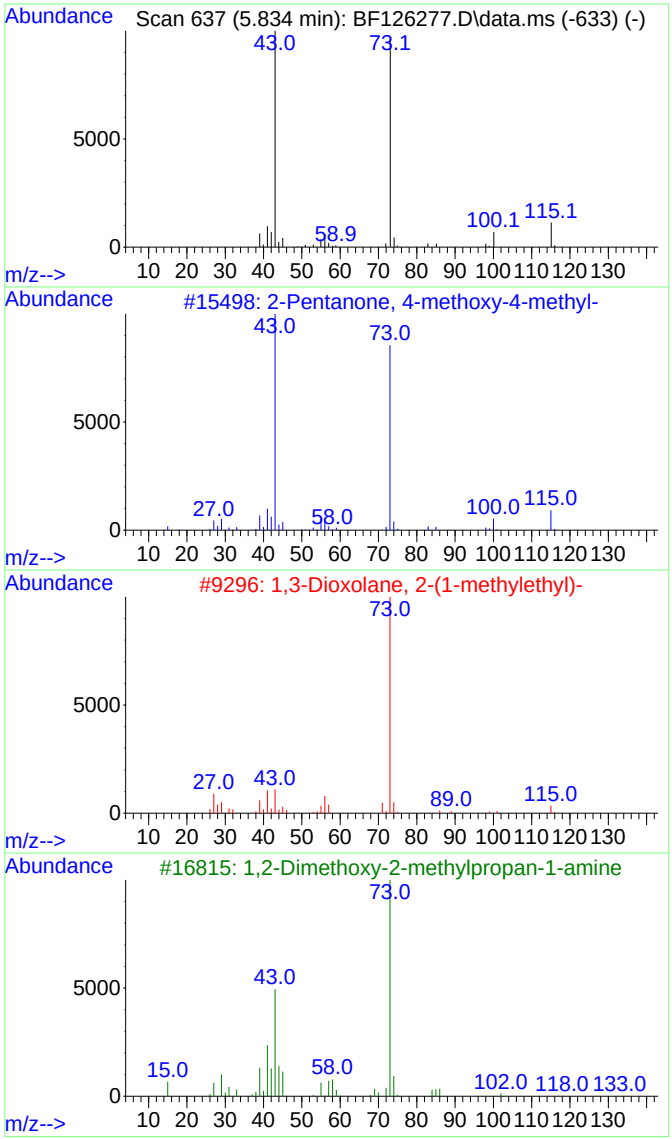
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

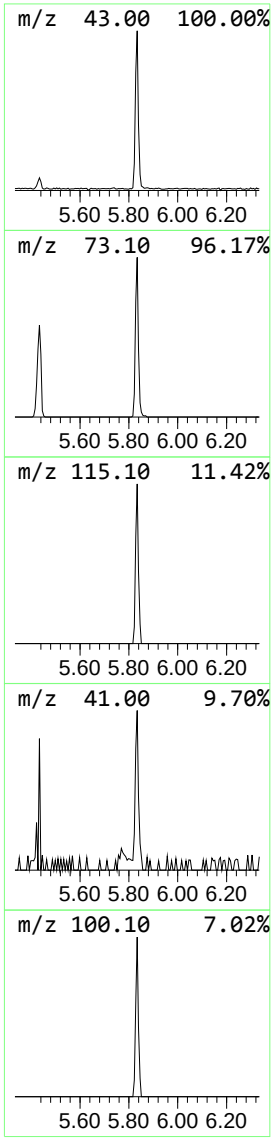
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	2.86 ng	116567	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	72
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	17
3	1,2-Dimethoxy-2-methylpropan-1-a...	133	C6H15NO2	1000445-17-2	17
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	12
5	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10





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

TIC Library : C:\Database\NIST20.L
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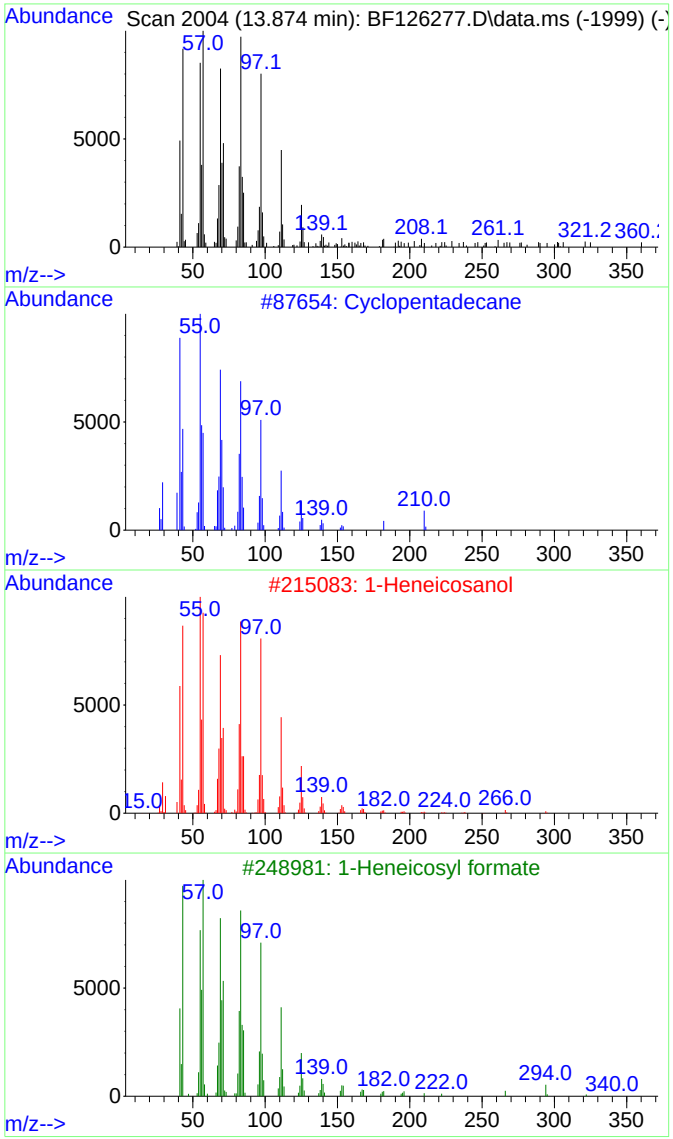
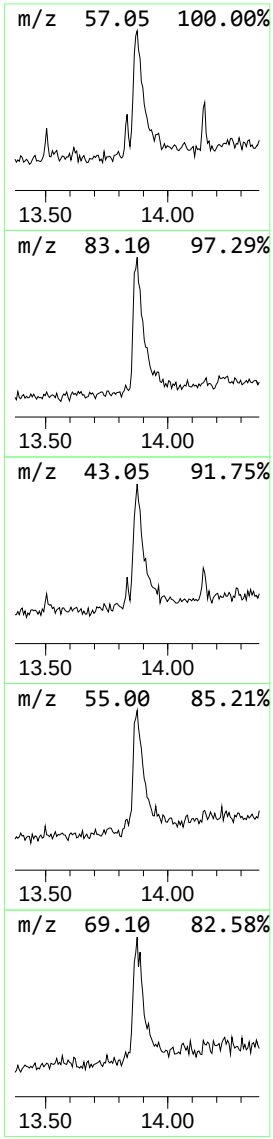
****

Peak Number 5 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	12.02 ng	518480	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	98
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
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TIC Library : C:\Database\NIST20.L
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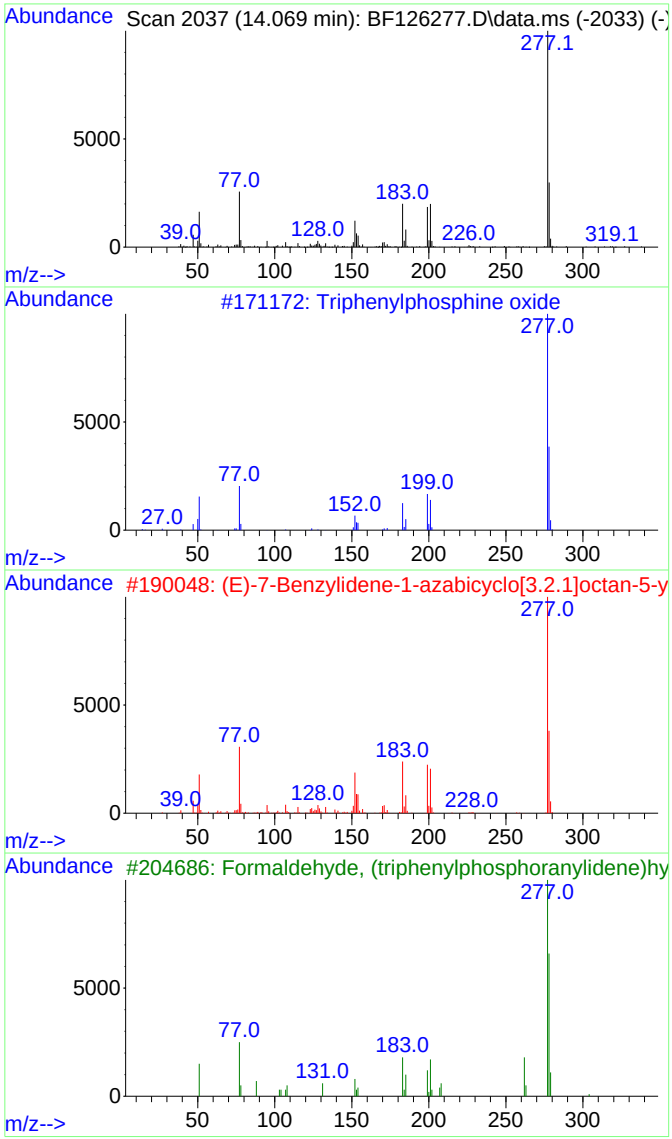
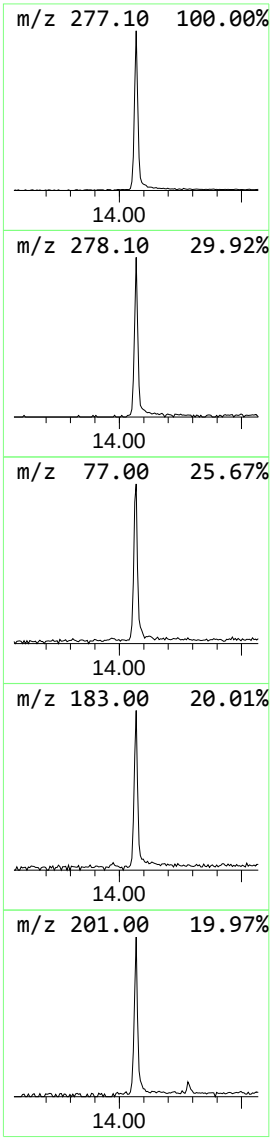
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.069	8.75 ng	377359	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	76
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	72
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	40





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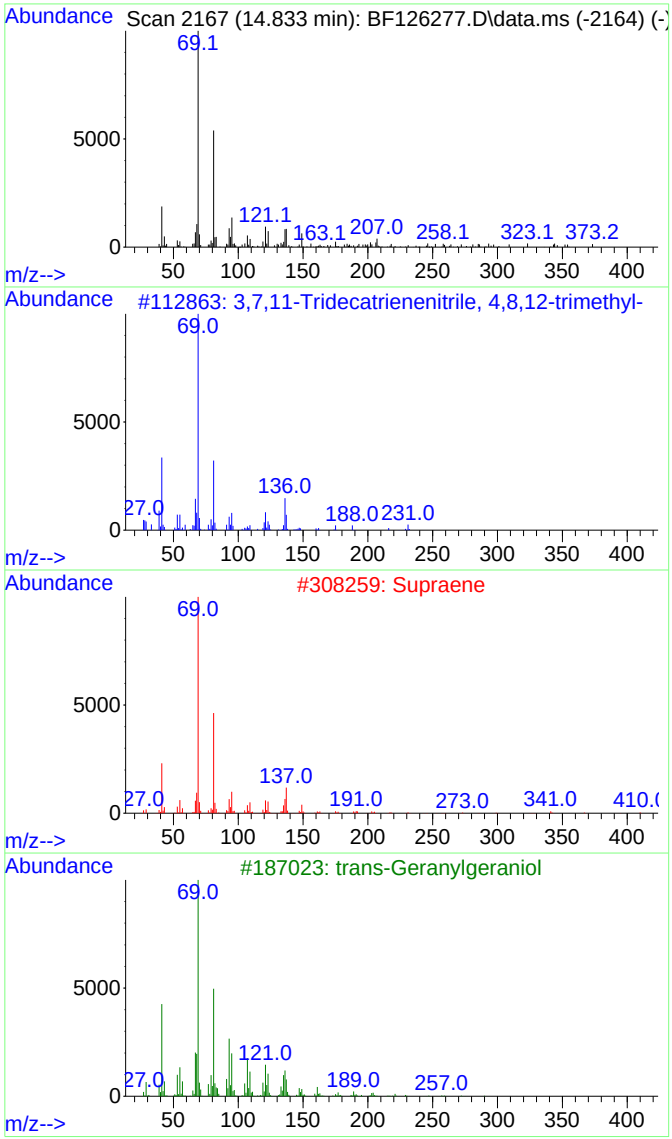
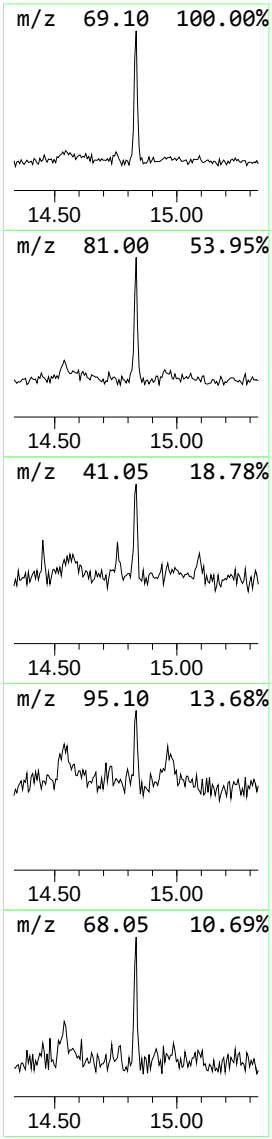
****
Peak Number 7 3,7,11-Tridecatrienenitrile... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.44 ng	108478	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
2	Supraene	410	C30H50	007683-64-9	72
3	trans-Geranylgeraniol	290	C20H34O	024034-73-9	72
4	Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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...	2.116	17.0	ng	694476	1	6.816	815576	20.0
Propane, 1,1-di...	2.216	2.8	ng	113981	1	6.816	815576	20.0
2-Pentanone, 4-...	5.028	28.1	ng	1145540	1	6.816	815576	20.0
2-Pentanone, 4-...	5.834	2.9	ng	116567	1	6.816	815576	20.0
Cyclopentadecane	13.874	12.0	ng	518480	5	13.974	862341	20.0
Triphenylphosph...	14.069	8.8	ng	377359	5	13.974	862341	20.0
3,7,11-Tridecat...	14.833	2.4	ng	108478	6	15.421	889953	20.0