LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005527.D
Acq On : 13 May 2021 19:27
Operator : CG/JU
Sample : M2371-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : VNJ-206

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_P\Methods\8270E-BP050521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005527.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.281	365	373	387	rBV	341139	487217	42.96%	9.275%
2	6.887	639	646	661	rBV	293829	466283	41.12%	8.877%
3	7.687	775	782	789	rVB	64077	97837	8.63%	1.863%
4	8.857	971	981	988	rBV	193152	318454	28.08%	6.062%
5	10.475	1247	1256	1270	rBV	64585	112963	9.96%	2.151%
6	12.957	1670	1678	1689	rBV	515654	732196	64.56%	13.939%
7	13.804	1817	1822	1829	rBV	44613	71960	6.35%	1.370%
8	14.334	1906	1912	1920	rBV	90340	138910	12.25%	2.644%
9	15.192	2050	2058	2061	rBV8	6128	12159	1.07%	0.231%
10	15.839	2161	2168	2177	rBV	495184	734768	64.79%	13.988%
11	17.092	2376	2381	2387	rBV	125636	183568	16.19%	3.495%
12	17.998	2530	2535	2545	rBV3	39842	65599	5.78%	1.249%
13	19.669	2813	2819	2826	rBV	939903	1134045	100.00%	21.589%
14	20.292	2921	2925	2929	rBV3	47162	58346	5.14%	1.111%
15	20.333	2929	2932	2938	rVB6	18551	25386	2.24%	0.483%
16	20.904	3026	3029	3036	rVB3	56101	83987	7.41%	1.599%
17	20.980	3039	3042	3048	rVB2	21819	27214	2.40%	0.518%
18	21.192	3073	3078	3084	rBV	166115	217989	19.22%	4.150%
19	21.804	3179	3182	3192	rVB8	33304	57251	5.05%	1.090%
20	23.504	3465	3471	3478	rVB2	116422	226719	19.99%	4.316%

Sum of corrected areas: 5252851

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
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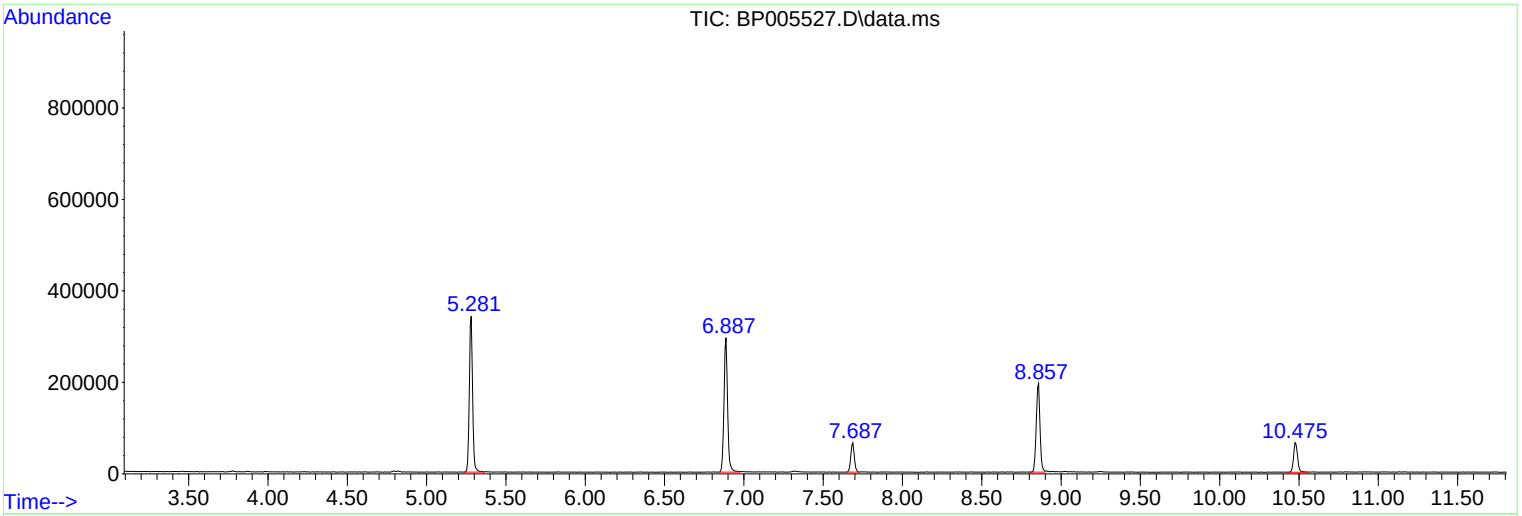
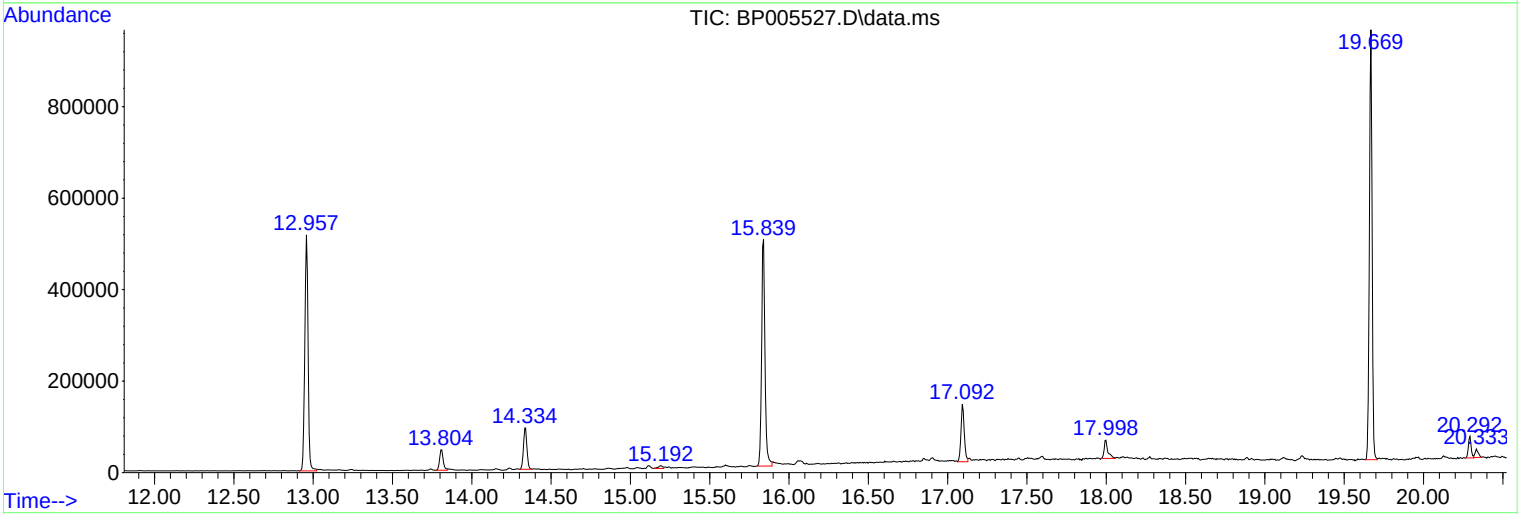
Sample : M2371-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

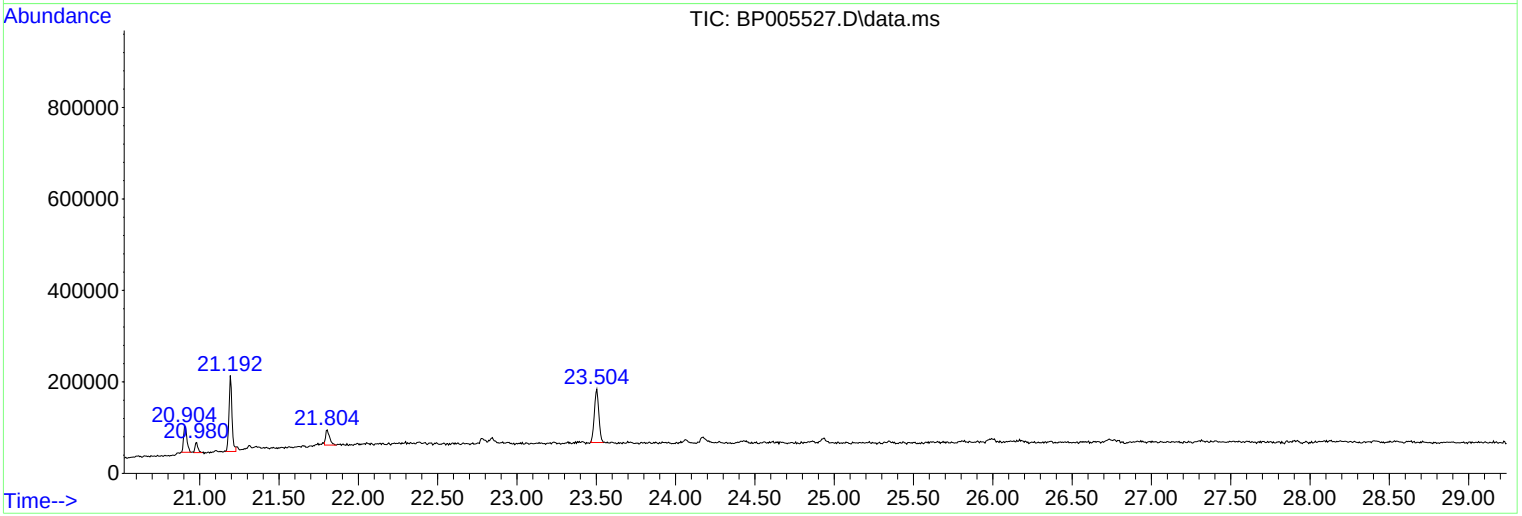
Instrument :
BNA_P
ClientSampleId :
VNJ-206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : BP005527.D
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Operator : CG/JU
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
VNJ-206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

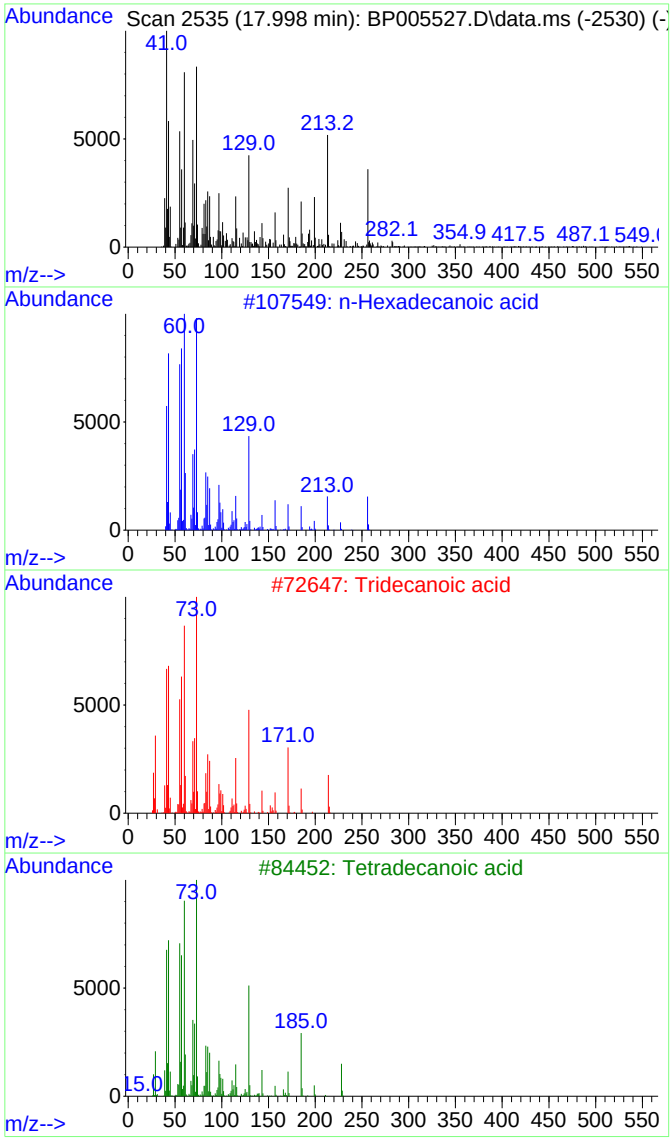
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

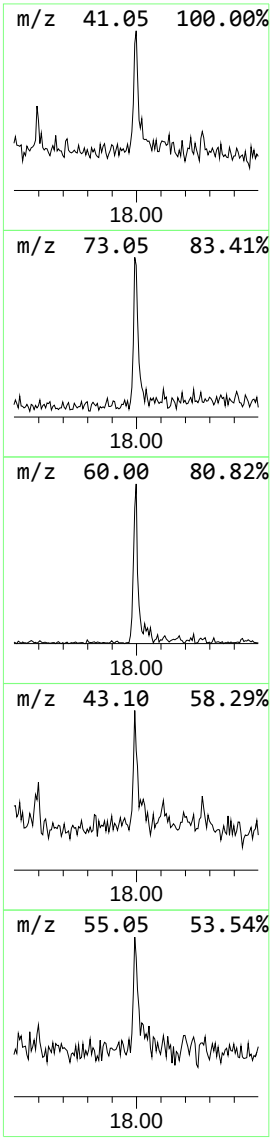
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.998	7.15 ng	65599	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tridecanoic acid	214	C13H26O2	000638-53-9	60
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	Dodecanoic acid	200	C12H24O2	000143-07-7	43
5	Undecanoic acid	186	C11H22O2	000112-37-8	41





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Data File : BP005527.D
Acq On : 13 May 2021 19:27
Operator : CG/JU
Sample : M2371-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : VNJ-206

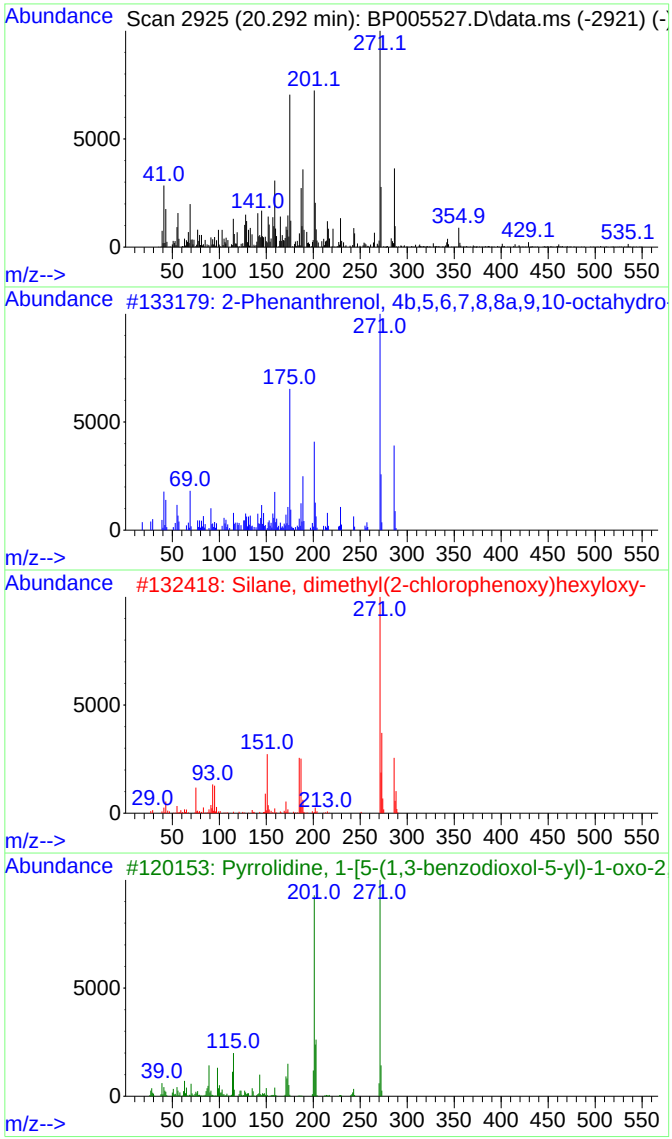
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

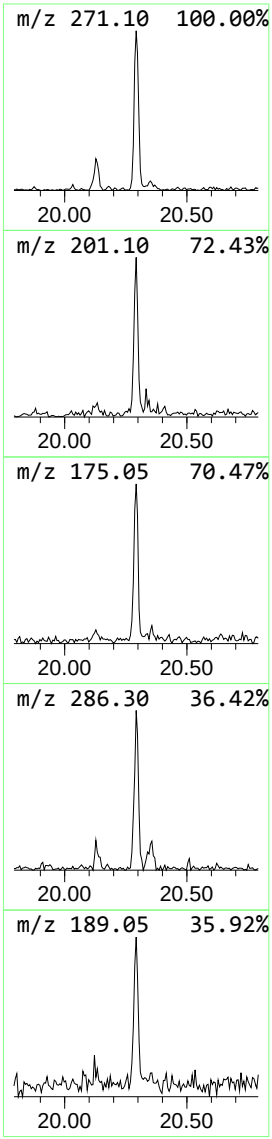
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.292	5.35 ng	58346	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	93
2	Silane, dimethyl(2-chlorophenoxy...	286	C14H23ClO2Si	1000347-07-3	46
3	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	43
4	Crinan-1-ol, 2,3-didehydro-,(1.a...	271	C16H17NO3	1000111-31-3	38
5	13-Isopropylpodocarpen-12-ol-20-al	300	C20H28O2	024035-37-8	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005527.D
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Operator : CG/JU
Sample : M2371-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
VNJ-206

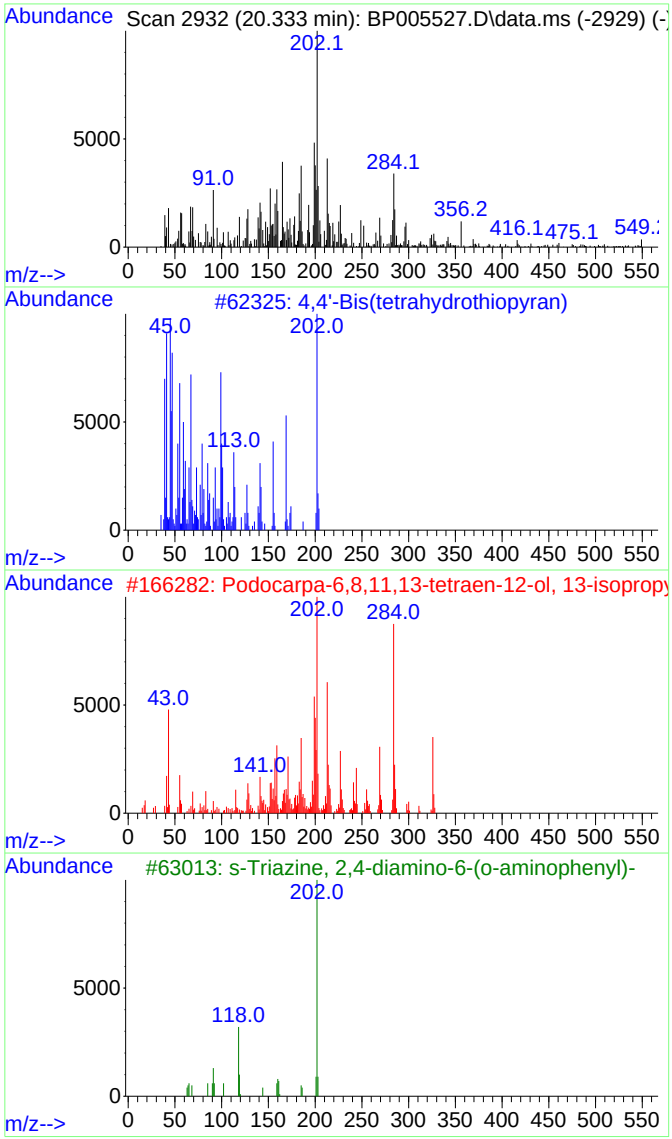
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

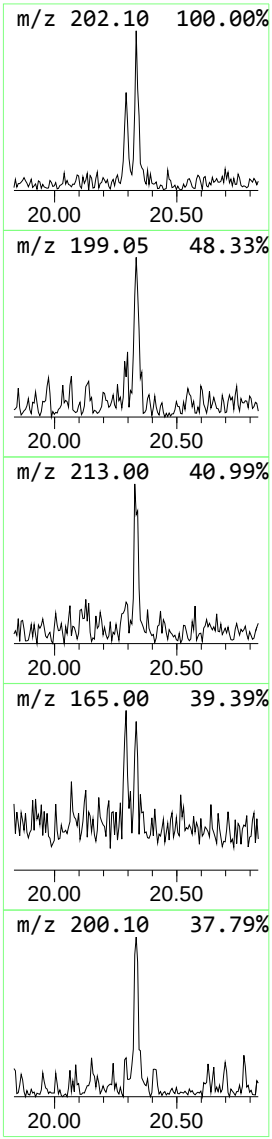
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.333	2.33 ng	25386	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	91
2	Podocarpa-6,8,11,13-tetraen-12-o...	326	C22H30O2	022160-86-7	62
3	s-Triazine, 2,4-diamino-6-(o-ami...	202	C9H10N6	029366-74-3	18
4	2-(para-Chlorobenzyl)-pyridine	203	C12H10ClN	004350-41-8	18
5	1-Naphthalenecarboxylic acid, 2-...	202	C12H10O3	000947-62-6	14





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Sample : M2371-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : VNJ-206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

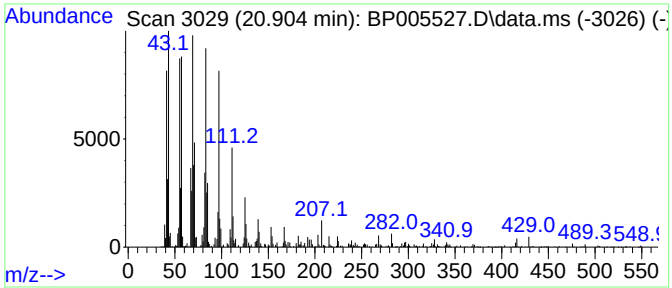
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

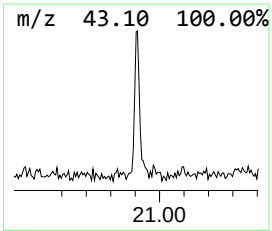
****

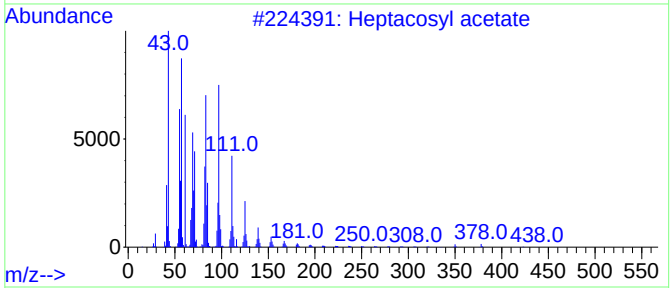
Peak Number 4 Heptacosyl acetate Concentration Rank 1

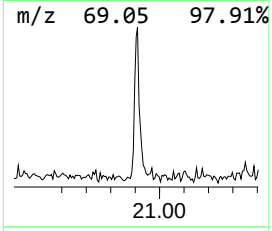
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.904	7.71 ng	83987	Chrysene-d12	21.192

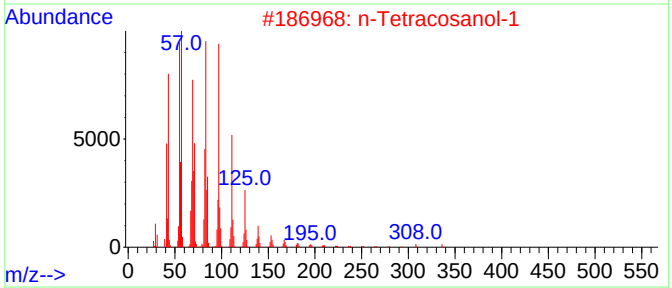
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl acetate	438	C29H58O2	1000351-78-2	92
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	1-Nonadecene	266	C19H38	018435-45-5	90
4	1-Triacontanol	438	C30H62O	000593-50-0	90
5	Triacontyl acetate	480	C32H64O2	041755-58-2	89

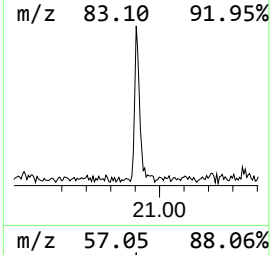


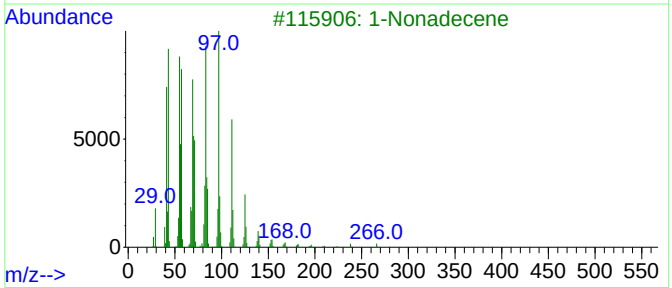


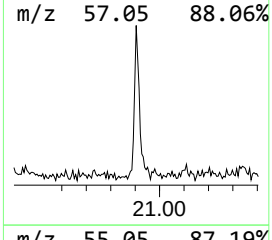


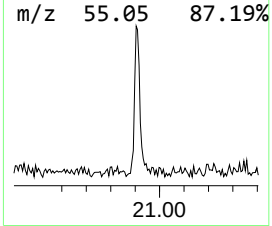












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Sample : M2371-01
Misc :
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Instrument :
BNA_P
ClientSampleId :
VNJ-206

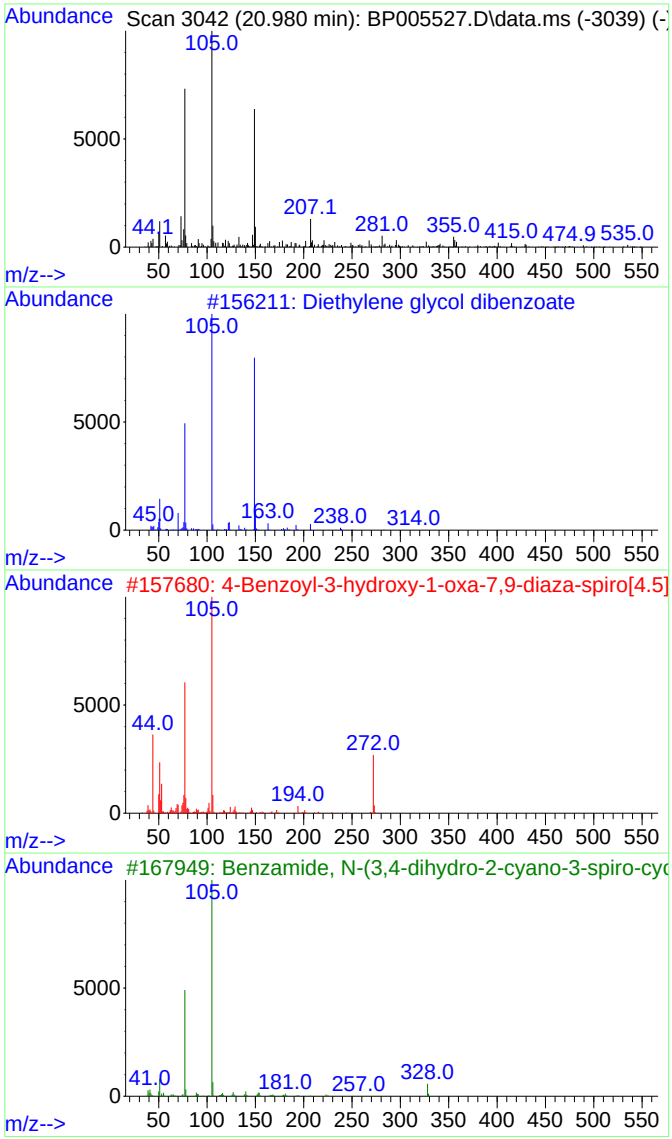
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

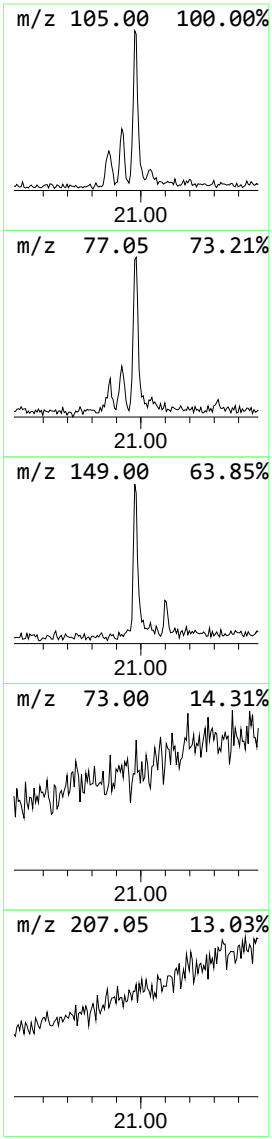
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	2.50 ng	27214	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2	4-Benzoyl-3-hydroxy-1-oxa-7,9-di...	316	C14H8N2O7	1000297-32-5	43
3	Benzamide, N-(3,4-dihydro-2-cyan...	328	C22H20N2O	136819-71-1	43
4	Benzeneacetic acid, .alpha.-hydr...	256	C16H16O3	052182-15-7	43
5	Benzoylformic acid	150	C8H6O3	000611-73-4	43





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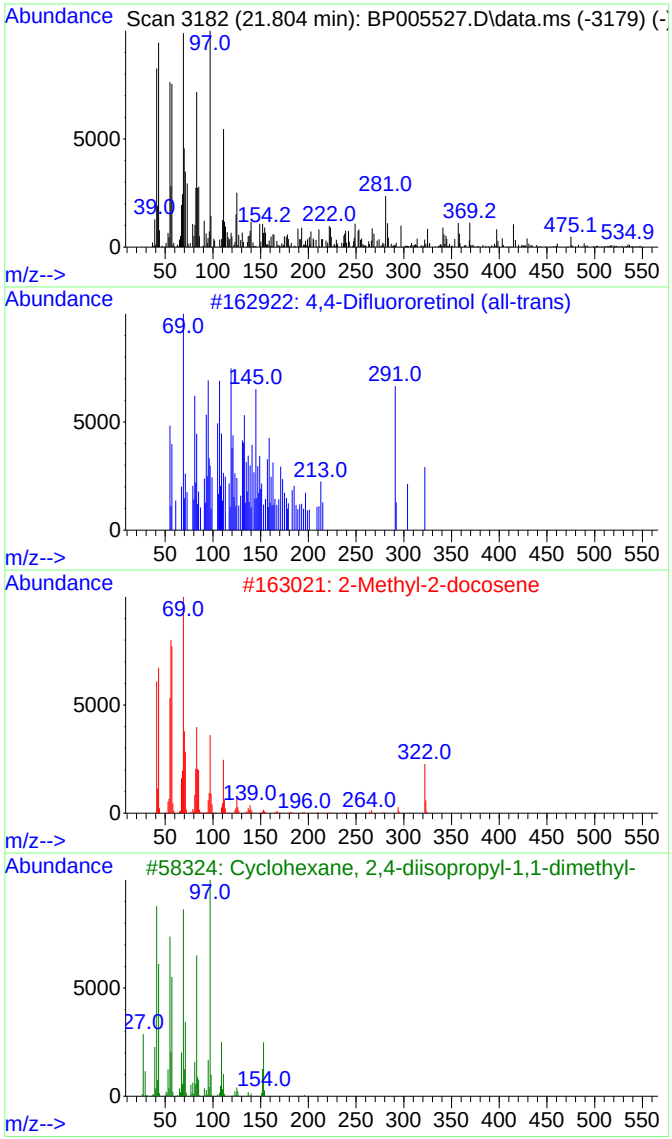
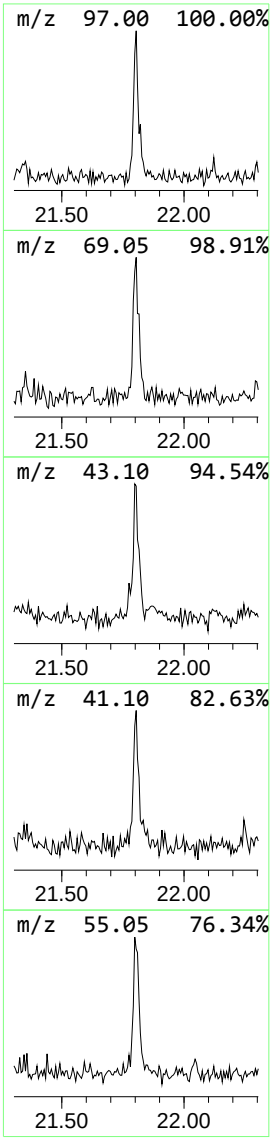
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4,4-Difluororetinol (all-tr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.804	5.25 ng	57251	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4-Difluororetinol (all-trans)	322	C20H28F2O	090660-21-2	93
2	2-Methyl-2-docosene	322	C23H46	1000131-16-9	83
3	Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	70
4	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	62
5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	55





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	17.998	7.2	ng	65599	4	17.092	183568	20.0
2-Phenanthrenol...	20.292	5.3	ng	58346	5	21.192	217989	20.0
4,4'-Bis(tetrah...	20.333	2.3	ng	25386	5	21.192	217989	20.0
Heptacosyl acetate	20.904	7.7	ng	83987	5	21.192	217989	20.0
Diethylene glyc...	20.980	2.5	ng	27214	5	21.192	217989	20.0
4,4-Difluororet...	21.804	5.3	ng	57251	5	21.192	217989	20.0